



Book of Abstracts

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# International Conference on Resource Chemistry - ICRC 2024

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## Welcome Statement

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### **Welcome to the ICRC 2024 - International Conference on Resource Chemistry at Fraunhofer IWKS!**

The increasing activity in resource chemistry, recycling, sustainable materials design, hydrogen etc. peaks every year - an exciting mix of applied and basic research captures the extraordinary progress in resource chemistry.

The aim of the conference is to assemble scientists from universities, scientific institutes as well as industry to promote international co-operations on sustainable materials development.

The conference will provide a forum for discussions among chemists, physicists, and materials scientists working with recycling technologies, substitution materials and design for and from recycling .

We are looking forward to fruitful discussions and an interesting meeting and hope that you enjoy the conference in the beautiful town of Alzenau.

Best Regards

Prof. Dr. Anke Weidenkaff  
Director Fraunhofer IWKS

## About Fraunhofer IWKS



Fraunhofer IWKS Location Hanau, Hesse



Fraunhofer IWKS Location Alzenau, Bavaria

>20  
current  
research  
projects

### Technologies for a world without waste

The **Fraunhofer Research Institution for Materials Recycling and Resource Strategies IWKS** develops circular materials and materials science technologies for an ultimate sustainable, waste-free circular economy. In close cooperation with universities, institutes

**As part of Fraunhofer Gesellschaft**, we aim to transfer scientific findings about key future-relevant technologies in industry and business and therewith contribute to the industrial transformation and a healthy planet.

**Fraunhofer IWKS aims to contribute to a sustainably healthy planet.** Its research focuses on establishing a closed circular economy: today's waste is tomorrow's resource. Valuable raw materials can be recovered and recycled or replaced by sustainable, environmentally and socially compatible alternatives. For this purpose, innovative processes are being developed in the fields of magnetic materials, energy materials, bioeconomics as well as digitalisation of resources.. The results of the research are transferred to industry.

>70  
employees



>50  
publications  
in 2023

and industry partners, it performs research on more sustainable alternatives for critical raw materials and elaborate solutions for an intelligent regeneration of innovative materials and their energy-efficient recovery.

The Fraunhofer IWKS team researches and works at two locations: Alzenau, Bavaria and Hanau, Hesse. With more than 70 employees from the fields of environmental management, process engineering, materials science, industrial engineering, (micro) biology, ecotrophology, chemistry and physics, the institute relies on an interdisciplinary research approach.

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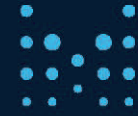
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# Conference Program



**ICRC 2024**  
International Conference  
on Resource Chemistry

## Monday, 11<sup>th</sup> March 2024

08:00 – 09:00 Registration

09:00 – 09:30 **Welcome Statement:** Prof. Dr. Anke Weidenkaff, Fraunhofer IWKS, Conference Chair  
Moderation: Dr. Gert Homm, Fraunhofer IWKS

09:30 – 10:00 **Keynote:** Dr. Stephan Andreas Schunk, hte GmbH & BASF SE  
Where do we stand in the Digital Transformation R&D Related to Materials Sciences?

10:00 – 10:10 Q&A

10:10 – 10:25 *Coffee break*

10:25 – 12:45 **Session 1 - Green Materials Synthesis, Sustainable Materials Development and Circular Economy**

Symposium Organizer, Session Chair: PD Dr. Emanuel Ionescu

10:25 Prof. Dr. Sanjay Mathur, University of Cologne (IS)  
Challenges of Greener Processing of Energy Harvesting Materials

10:50 Prof. Dr. Silvia Gross, University of Padova (IS)  
Enabling circular economy: the overlooked role of inorganic materials chemistry

11:15 Prof. Dr. Christoph Helbig, Universität Bayreuth (IS)  
Materials for future – resilient, recycled, carbon neutral

11:40 – 11:55 *Coffee break*

11:55 Dr. Philipp Walter, Heraeus Precious Metals GmbH & Co.KG (IS)  
Overview on Circularity for PEM Technologies – The Past, the Now and the Future

12:20 Dr. Steffi Weyand, Fraunhofer IWKS (IS)  
Advancing prospective life cycle assessment to support the development of innovative and more circular materials

12:45 PD Dr. Emanuel Ionescu (CS)  
Structural and Functional Ceramic Nanocomposites for Applications in Harsh Environmental Conditions

13:00 – 13:45 *Lunch*

IS = Invited Speaker  
CS = Contributed Speaker

# Conference Program



**ICRC 2024**  
International Conference  
on Resource Chemistry



## Monday, 11<sup>th</sup> March 2024

### 13:45 – 16:25 **Session 2 - Materials for Sustainable Cooling Applications**

Symposium Organizers: Dr. Wenjie Xie, Jürgen Gassmann, Fraunhofer IWKS  
Session Chair: Prof. Dr. Oliver Gutfleisch, TU Darmstadt

13:45 Dr. Franziska Scheibel, TU Darmstadt (IS)  
Magneto- and Multicaloric Materials from Basic Mechanism to Application

14:10 Falk Münch, MAGNOTHERM Solutions GmbH (IS)  
Cooling with magnets – Bringing the cooling industry to the 21st century

14:35 Dr. Pingjun Ying, Leibniz Institute for Solid State and Materials Research (IS)  
A robust thermoelectric module based on  $\text{MgAgSb}/\text{Mg}_3(\text{Sb}, \text{Bi})_2$  with a conversion efficiency of 8.5% and a maximum cooling of 72 K

15:00 Prof. Dr. Armin Feldhoff, Leibniz University Hannover (IS)  
Thermoelectric cooling - The prospects of calcium cobaltate as p-type component in an efficient entropy pump

### 15:25 – 15:45 *Coffee break*

15:45 Dr. Andrey Kovalevsky, University of Aveiro (IS)  
Thermoelectrics for Sustainable Future: The Case of Strontium Titanate

16:10 Chi-Chia Lin, Fraunhofer IWKS (CS)  
Enhancing magnetic properties and rare earth element utilization efficiency of Ce-containing Nd-Fe-B magnets by the 2-powder method

### 17:00 **Postersession and Networking Dinner**

IS = Invited Speaker  
CS = Contributed Speaker

# Conference Program



**ICRC 2024**  
International Conference  
on Resource Chemistry



## Tuesday, 12<sup>th</sup> March 2024

### 08:30 – 11:35 **Session 3 - Green Materials for Green Hydrogen**

Session Chair, Symposium Organizer: Dr. Till Frömling, Fraunhofer IWKS  
Symposium Organizers: Andreas Brumby, Materials Valley e. V.  
Dr. Marc Widenmeyer, TU Darmstadt

08:30 Prof. Dr. Ulrike Kramm, TU Darmstadt (IS)  
How rethinking the chemistry of iron can contribute to a more sustainable future

08:55 Dr. Steffen Hasenzahl, Evonik Operations GmbH Creavis (IS)  
Successful development and scale-up of materials as pre-condition for a climate-neutral hydrogen economy

09:20 Dr. Thomas Fischer, University of Cologne (IS)  
On the Way to Sustainable Hydrogen: Visions and Limitations of Photoelectrochemical Water Splitting Technologies

09:45 Andreas Brumby, Materials Valley e. V. (IS)  
Critical Raw Materials for the Hydrogen Economy

### 10:10 – 10:25 *Coffee break*

10:25 Prof. Dr. Ümit Demirci, European Institute for Membranes & University Montpellier (IS)  
BN(C)H materials for hydrogen storage and production

10:50 Nikita Gugin, Bundesanstalt für Materialforschung und -prüfung (BAM) (CS)  
Large-Scale Green Synthesis of a Model BSA@ZIF-8 Biocomposite via Reactive Extrusion

11:05 Dr. Andreas Hertwig, Bundesanstalt für Materialforschung und -prüfung (BAM) (CS)  
New analytic ways to characterise mesoporous thin layers used in electrocatalytic water splitting

IS = Invited Speaker  
CS = Contributed Speaker

# Conference Program



**ICRC 2024**  
International Conference  
on Resource Chemistry



## Tuesday, 12<sup>th</sup> March 2024

- 11:35 – 12:05 **Keynote:** Prof. Dr. Bilge Yildiz, Massachusetts Institute of Technology, USA  
Controlling Metal Nanoparticle Exsolution on Oxides By External Drivers – Defects, Elastic Strain and Ion Irradiation
- 12:05 – 12:15 Q&A
- 12:15 – 13:15 *Lunch*
- 13:15 – 16:45 **Session 4 - Green Batteries**  
Symposium Organizer, Session Chair: Dr. Benjamin Balke-Grünewald, Fraunhofer IWKS
- 13:15 Dr. Guinevere Giffin, Fraunhofer ISC (IS)  
Sustainable production & recycling of green batteries
- 13:45 Prof. Dr. Emma Kendrick, University of Birmingham (IS)  
Designing sustainability into new battery chemistries
- 14:10 Dr. Magdalena Graczyk-Zajac, EnBW (IS)  
Towards sustainable, grid connected stationary storage system: ResHy project
- 14:35 – 14:50 *Coffee break*
- 14:50 Prof. Dr. Monika Wilamowska-Zawlocka, Gdansk Polytechnic University (IS)  
Challenges of direct recycling of used lithium-ion batteries
- 15:15 Dr. Songhak Yoon, Fraunhofer IWKS (IS)  
How to revitalize the spent lithium-ion batteries
- 15:40 **Postersession and Networking**
- 18:00 **Conference Dinner and Poster awards**

IS = Invited Speaker  
CS = Contributed Speaker

# Conference Program



**ICRC 2024**  
International Conference  
on Resource Chemistry



## Wednesday, 13<sup>th</sup> March 2024

- 09:30 – 10:00 **Keynote:** Prof. Dr. Claudia Felser, Max Planck Institute for Chemical Physics of Solids  
Topology for energy efficient spintronics and energy conversion
- 10:00 – 10:10 Q&A
- 10:10 – 10:20 *Coffee Break*
- 10:20 – 12:25 **Session 5 - Plasma-assisted CO<sub>2</sub> (&H<sub>2</sub>) Utilization**  
Symposium Organizer: Dr. Marc Widenmeyer, TU Darmstadt  
Session Chairs: Dr. Marc Widenmeyer, Dr. Andreas Schulz, University of Stuttgart
- 10:20 Prof. Dr. Xin Tu, University of Liverpool (IS)  
Plasma catalysis: A promising solution for decentralized production of fuels and chemicals
- 10:45 Dr. Andreas Schulz, University of Stuttgart (IS)  
Activation of low-energy molecules using the example of CO<sub>2</sub> in microwave air plasmas
- 11:10 Dr. Amandine Guissart, Muegge GmbH (IS)  
Microwave Plasma Sources for Sustainable Applications
- 11:35 Dr. Marc Widenmeyer, TU Darmstadt (IS)  
Merging Materials Performance and Sustainability: Ceramic Oxygen Transport Membrane Materials as an Exemplar
- 12:00 Dr. Thomas Schiestel, Fraunhofer IGB (IS)  
MIEC hollow fiber membranes for the separation of oxygen from a CO<sub>2</sub> plasma
- 12:25 – 13:15 *Lunch*

IS = Invited Speaker  
CS = Contributed Speaker



# Conference Program



**ICRC 2024**  
International Conference  
on Resource Chemistry

## Wednesday, 13<sup>th</sup> March 2024

### 13:15 – 16:10 **Session 6 - Chemical Recycling of Plastics**

Symposium Organizers: Dr. Gert Homm, Fraunhofer IWKS  
Dr. Marc Widenmeyer, TU Darmstadt  
Session Chair: Prof. Dr. Xin Tu, University of Liverpool

13:15 Dr. Yeshui Zhang, University of Aberdeen  
Advanced Metrology for Studying Catalyst Degradation & Li-ion Battery Drying Process (IS)

13:45 Dr. Holger Helten, University Würzburg  
Furan-based optoelectronic materials from renewable resources – a successful example where sustainability and performance go hand in hand (IS)

14:05 Prof. Dr. Martin Gräbner, TU Bergakademie  
Overview on thermo-chemical Conversion Processes for Chemical Recycling (IS)

14:30 Prof. Dr. René Wilhelm, TU Clausthal (IS)  
Chemical Recycling of Carbon Fiber Composites

### 14:55 – 15:15 *Coffee break*

15:15 Prof. Dr. Bert Weckhuysen, Utrecht University (IS)  
Challenges, Opportunities and Some Mechanistic Understanding in the Chemical Recycling of Plastic Waste

15:40 Tomislav Stolnar, Bundesanstalt für Materialforschung und -prüfung (BAM) (CS)  
Upcycling waste PET bottles to porous UiO-66 by mechanochemistry

15:55 Xiaio Yu, Fraunhofer IWKS (CS)  
Chemical recycling of medical plastic waste over perovskite-type catalysts for hydrogen production

### 16:10 **Closing remarks**

IS = Invited Speaker  
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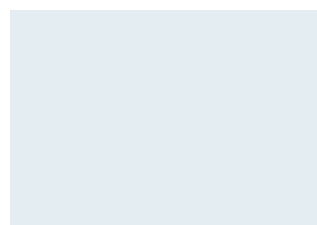


# I. Keynotes

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Dr. Stephan Andreas Schunk

## Where do we stand in the Digital Transformation R&D Related to Materials Sciences?



*Dr. Stephan Andreas Schunk  
hte gmbh. BASF SE  
Universität Leipzig, Germany  
Institute for Chemical  
Technology*

Digital transformation efforts in academia and industry have become a trending topic within the last decade. The topic is branded as “Digitalization” and associated to the high-tech agendas of leading enterprises and academic organizations seeking to embrace the potential of change. The four guiding principles which are the core elements that are addressed within the context of industry 4.0 are interoperability, information transparency, technical assistance, and decentralized decisions. It is not self-evident how these principles can have an impact on research and development in both environments: industrial and academic. Natural sciences, and especially chemistry, are science disciplines with a strong tradition and are based on knowledge about chemicals and materials, physical chemistry as foundation and as experimental sciences follow the traditional canon of experimentation together with resulting experimental evidence and interpretation of the obtained results. In the era of digital transformation given the fact of an increased availability of data together with improved modelling capacities, the potential to predict behavior of complex chemical systems and the opportunity to do more targeted experimental work with an increased amount of fully automated and integrated devices the traditional workflows followed in R&D can be questioned – do these traditional models still fit to the digital transformation that industry and academia are targeting at? Can or should R&D be decoupled from digitalization – and what will be the role of academia within the context?

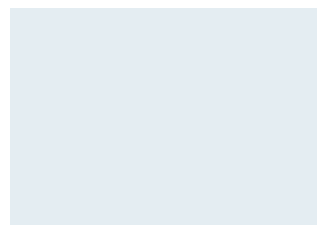
The lessons learned up to now in both, academia and industry can help in many aspects to further accelerate the digital transformation efforts within research and development in materials sciences – in both: academia and industry. Apart from common standards used throughout the communities to enable machine readability of data, access to experimental data of measurable of high quality are two of the core elements, which allow the assessment of chemical properties through an integrated data view and enhanced by modern data analysis methods with high efficiency. Nevertheless, one of the major challenges that still must be worked on is the closure of the information cycle to the disciplines dealing with theoretical approaches in materials sciences. The oral contribution will focus on demands of digital approaches materials sciences and also which approaches can be taken in the materials science arena as a community of practice to arrive at a state where theory and practice can work synergistically through digitalization.

# I. Keynotes

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Prof. Dr. Bilge Yildiz

## Controlling Metal Nanoparticle Exsolution on Oxides By External Drivers – Defects, Elastic Strain and Ion Irradiation



*Prof. Dr. Bilge Yildiz  
Massachusetts Institute of  
Technology, USA*

Exsolution is an effective approach to fabricating oxide-supported metal nanoparticle (electro-) catalysts via phase precipitation out of a host oxide. A fundamental understanding and control of the exsolution kinetics are needed to engineer the size, density and composition of exsolved nanoparticles to obtain higher catalytic activity toward clean energy and fuel conversion reactions, such as in solid oxide fuel and electrolysis cells. Since oxygen release via oxygen vacancy formation in the host oxide is behind oxide reduction and metal exsolution, we hypothesize that the kinetics of metal exsolution should depend on the kinetics of oxygen release. In this work, we probe the surface exsolution kinetics both experimentally and theoretically using thin-film perovskite oxide model systems, show its relation to the oxygen evolution kinetics, and tune it by external drivers including elastic strain and ion irradiation. Using both drivers, we couple to the formation of point defects and defect clusters, that serve as nucleation sites for nanoparticle exsolution. As a result, we can controllably tune size, density, composition and position of the exsolved metal nanoparticles. This findings can guide the design of exsolution electrocatalysts to advance the performance and durability of solid oxide electrochemical cells.

# I. Keynotes

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Prof. Dr. Claudia Felser

## Topology for energy efficient spintronics and energy conversion



Prof. Dr. Claudia Felser  
Max Planck Institute for Chemical Physics of Solids

Topology, a mathematical concept, recently became a hot and truly transdisciplinary topic in condensed matter physics, solid state chemistry and materials science. All 200 000 inorganic materials were recently classified into trivial and topological materials, such as topological insulators, Dirac, Weyl and nodal-line semimetals, and topological metals [1]. More than 25% of all materials host topological bands around the Fermi energy. Beyond the single particle picture, we have identified first antiferromagnetic topological materials [2]. Experimentally, we have realized ferromagnetic materials, examples are  $\text{Co}_2\text{MnGa}$  and  $\text{Co}_3\text{Sn}_2\text{S}_2$ . Surprisingly all crossings in the band structure of ferromagnets are Weyl nodes or nodal lines [3].  $\text{Mn}_3\text{Sn}$  and  $\text{YbMnBi}_2$  are examples of non collinear antiferromagnetic Weyl semimetals, which show giant values for the anomalous Hall and Nernst effect [4]. Kagome lattice even beyond  $\text{Co}_3\text{Sn}_2\text{S}_2$  and  $\text{Mn}_3\text{Sn}$  have tunable properties based on the unique band structure with van Hove singularities, Weal points and flatbands. There is a large class of materials of the composition 1:6:6 ( $\text{RE}_6\text{Z}_6$  RE=rare earth, T=transition metal, Z=main group metal), which allows a flexible design of the electronic structure additional to charge density wave instabilities. In the context of real space topology, skyrmions and antiskyrmions are a possible new direction for new data storage [5]. Our goal is to identify new quantum-materials for highly efficient spintronics, quantum computing and energy conversion.

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# Session I

Green Materials Synthesis, Sustainable Materials Development and Circular Economy

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**Prof. Dr. Sanjay Mathur**

## Challenges of Greener Processing of Energy Harvesting Materials



*Prof. Dr. Sanjay Mathur*  
*University Cologne, Germany*

Solution processed Perovskite Solar Cells (PSCs) are already leading the pack of leading photovoltaic technologies competing with inorganic thin-film solar cells and mainstream multi-crystalline silicon cells in terms of efficiency and production costs. However, there are a large number of materials challenges both in terms of composition (stability, toxicity, etc.) and device applications (endurance under in-operando conditions, hydrolysis, etc.) that still need to be addressed to realize the device potential of this promising class of materials. Besides greener approaches (lead-free compositions, non-toxic solvent, etc.), the desired maturity of PSC technology demands a judicious reduction of parametric space of materials synthesis and selection of materials based on their limited stress-tolerance (e.g., ion migration) and resilience under processing and operational conditions. In this context, the main objectives of greener or alternative processing are to solve two major issues associated with the implementation of PSCs; toxicity and stability. Most of the PSC fabrication is done utilizing dimethyl formamide (DMF) as the solvent that is listed among "Substances of very high concern" by the European Chemical Agency and its use may represent a potential hurdle for the future industrial production of the perovskite-based PV technology. Another major toxic component is its metal (Pb) part. The toxicity of the water-soluble source of lead remains as another limitation in outdoor application of these types of solar cells. In general, replacing Pb with other less or non-toxic metals remains a challenge.

This talk will address the challenges associated with alternative and greener processing of photon harvesting materials.

# Session I

Green Materials Synthesis, Sustainable Materials Development and Circular Economy

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**Prof. Dr. Silvia Gross**

## **Enabling circular economy: the overlooked role of inorganic materials chemistry**



*Prof. Dr. Silvia Gross  
University of Padova, Italy  
KIT Karlsruhe, Germany*

The currently prevalent productive system is based on a “take–make–dispose” logic, which assumes that energy and resources are unlimited, available, and easy to dispose of. This linear economy approach is no longer sustainable in the global context, due to the sharply increasing exploitation of non-renewable resources and the consequent growing degradation of our planet. A viable alternative is the one proposed and redesigned in a coherent context by Ellen MacArthur who, since the early 2000s, coined the expression “circular economy” as a possible answer to the limited availability of necessary resources, both materials and energy ones. The pivotal role of chemistry in this context is well acknowledged, but it is typically explained as the role of molecular chemistry through the concept of “circulating molecules”, that is, re-using and recycling existing molecules that are the building blocks of the end-consumer products approaching the end of their lives. However, inorganic non-molecular materials, such as ceramics, metals, alloys, semi-conductors, etc. constitute the majority of solid materials and play key roles as construction materials, and for industries such as automotive, microelectronics, lighting or as materials for regenerative and sustainable energy conversion and storage. Therefore, circular approaches for these classes of materials are of high importance. Specifically relevant is inorganic chemistry, encompassing both molecular and materials/solid state aspects.

# Session I

Green Materials Synthesis, Sustainable Materials Development and Circular Economy

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**Prof. Dr. Christoph Helbig**

## **Materials for future – resilient, recycled, carbon neutral?**



*Prof. Dr. Christoph Helbig  
University of Bayreuth,  
Germany*

To count as “sustainable,” materials nowadays must fulfill many aspects. We want them to be safe for people and the planet, free of criticality and conflict, fully circular in the global economy, and carbon neutral. Of course, we still want them to have high performance and enable long product lifetime. Hardly can all these requests be fulfilled equally and free of cost, but they need to be addressed. Therefore, evaluating the full sustainability potential of new materials requires a broad knowledge and expertise in various assessment methods, combined with the courage to prioritize sustainability dimensions depending on the anticipated application of the material. This talk presents the current status of assessment methods for critical raw materials, circularity, and carbon footprint of materials, focusing on metals and raw materials. It further shows the need for improved data collection, essential fields for scientific collaboration, and options for integrating material sustainability into material selection and development procedures.



# Session I

Green Materials Synthesis, Sustainable Materials Development and Circular Economy

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**Dr. Philipp Walter**

## Overview on Circularity for PEM Technologies – The Past, the Now and the Future



*Dr. Philipp Walter*  
*Heraeus Precious Metals*  
*GmbH & Co.KG*

Precious Metals, in particular Platin Group Metals, are indispensable elements for the hydrogen economy. In particular for Proton Exchange Membrane (PEM) Electrolyzers and Fuel Cells, they are used as catalyst materials, but increasingly also as coating in PEM stacks to protect against corrosion or to increase the conductivity.

Whereas the high value of Precious Metals motivates for their recovery and recycling, other parts of PEM Electrolyzer and Fuel Cell Stacks are increasingly considered for recycling, too, due to various reasons.

The presentation highlights the state of the art of precious metals recycling from PEM Electrolyzers and Fuel Cells and gives an outlook into future recycling streams and materials.

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# Session I

Green Materials Synthesis, Sustainable Materials Development and Circular Economy

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Dr. Steffi Weyand

## Advancing prospective life cycle assessment to support the development of innovative and more circular materials



*Dr. Steffi Weyand  
Fraunhofer IWKS, Germany*

Sustainable materials are needed in application fields such as renewable energy or the chemical sector for the transition towards climate-friendly production. A sustainable material implies that in addition to its functional performance, the environmental performance needs to be assessed from a multi-criteria perspective. This is especially relevant for developing innovative and circular materials at early development stages when design freedom is still high.

Prospective life cycle assessment (p-LCA) supports the early-stage assessment of environmental impacts. P-LCA uses upscaling frameworks and scenario approaches to determine the future environmental performance of innovative technologies. Recent p-LCA frameworks have also considered material-specific aspects: the UpFunMatLCA proposes a systematic upscaling scheme for material development distinguishing between upscaling mechanisms for process learning, material learning, and external developments. Despite the availability of existing frameworks, few case studies have performed a systematic upscaling for innovative biobased, recycled, or alternative materials.

This research applies the systematic upscaling scheme UpFunMatLCA to a case study on the production of biobased binders and performs a p-LCA from lab/pilot to early fab scale. We demonstrate how the upscaling scheme can be integrated into the material development process and analyze the effects of the different upscaling mechanisms on future environmental performances. The results indicate a very high potential for environmental improvements from lab to early fab scale, driven by process learning and external developments. We critically discuss the feasibility of systematic upscaling and outline specifics for assessing recycled and more circular materials.

# Session I

Green Materials Synthesis, Sustainable Materials Development and Circular Economy

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PD Dr. Emanuel Ionescu

## Structural and Functional Ceramic Nanocomposites for Applications in Harsh Environmental Conditions



*PD Dr. Emanuel Ionescu  
Fraunhofer IWKS and  
Technische Universität Darm-  
stadt, Germany*

In the present talk, our recent activities related to the development of novel ceramic nanocomposites to be operated at high temperatures as well as in ultra-harsh environmental conditions will be highlighted and critically discussed. Typically, single-source precursors based on silicon-based polymers with tailor made molecular structure are used to preparatively access ceramic nanocomposite formulations showing excellent robustness against decomposition, devitrification, oxidation/corrosion and/or creep, which may be used as high-potential structural materials for internal combustion engines or in chemical plants. Additionally, the developed materials possess specific functionalities such as chemiresistive, temperature or strain sensing capability. The talk will exemplarily introduce materials developments related to e.g., novel ultrahigh-temperature ceramic coatings or piezoresistive strain sensors and will elaborate on the perspectives of precursor-based ceramic nanocomposites as highly promising functional materials for operation in extreme conditions

# Session II

## Materials for Sustainable Cooling Applications

Dr. Franziska Scheibel

### Magneto- and Multicaloric Materials from Basic Mechanism to Application



Dr. Franziska Scheibel  
Technische Universität Darmstadt, Germany

Cooling and refrigeration account for approximately 20% of global electricity demand and 8% of greenhouse gas emissions. Current vapor compression technology is inefficient and uses refrigerant gases with a high global warming potential. Magnetocaloric cooling is a solid-state cooling technology that uses the cyclic magnetization and demagnetization of solid-state magnetocaloric materials instead of high-GWP refrigerants. The application temperature depends on the class of magnetocaloric material used, and magnetocaloric cooling applications range from room temperature cooling to hydrogen liquefaction [1-4]. Good magnetocaloric materials exhibit high magnetization, large entropy, and adiabatic temperature changes. In addition to these fundamental material properties, secondary functionalities such as mechanical stability, cyclic performance, criticality, and non-toxicity are required, along with the fact that the material should be easy to form in a scalable process. In our research, we investigate several magnetocaloric and multicaloric materials for their caloric performance including the secondary functionalities and different scalable processing techniques to enable the development of magnetocaloric and multicaloric materials from basic mechanism to application.

A large caloric effect can be observed in the vicinity of the first order magnetostructural phase transitions in multi-caloric Ni-Mn based Heusler alloys. Using the material in a multi-stimulus cooling cycle (magnetic field and compressive stress) allows a large caloric effect under cyclic conditions [5]. By tailoring the chemical composition and microstructure, we were able to increase the mechanical stability for reliable cyclic performance combined with optimal thermal hysteresis width and large caloric effects [6-7]. A relatively new processing method for the microstructure design of Ni-Mn based Heusler alloys is additive manufacturing, which additionally meets the requirement of a scalable process including high flexibility for the geometric design [8,9]. For the development of magnetocaloric materials for hydrogen liquefaction, the tunable transition temperature of the alloy is essential due to the wide temperature range from 77K to 20K. Heavy rare-earth-based Laves phases exhibit a large MCE, but the criticality and abundance of the heavy rare earth elements need to be considered for applications. Therefore, we have investigated strategies to reduce the heavy-RE content while preserving the large MCE. This work was supported by the ERC Advanced Grant »CoolInnov« (No. 743116) and the CRC/TRR 270 »HoMMage« (DFG), and Helmholtz-RSF Joint Research Group (Project No. HRSF-0045).

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# Session II

Materials for Sustainable Cooling Applications

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Falk Münch

## Cooling with magnets – Bringing the the cooling industry to the 21st century



The global cooling industry accounts for over 10% of the global green house gas emissions and was only recently recognized as a major contributor to global warming in COP23. In my talk I will give an overview of the magnetic cooling technology, its fundamental principles and its benefits to our society. Furthermore, I will also highlight the importance of utilizing re-used/ recycled magnets and our recent progress with our cooling machines.

*Falk Münch*  
*MAGNOTERM Solutions GmbH*  
*Germany*

# Session II

## Materials for Sustainable Cooling Applications

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### Dr. Pingjun Ying

## A robust thermoelectric module based on MgAgSb/Mg 3 (Sb, Bi) 2 with a conversion efficiency of 8.5% and a maximum cooling of 72 K



*Dr. Pingjun Ying  
Leibniz Institute for Solid  
State and Materials Research  
Dresden, Germany*

The applications of thermoelectric (TE) technology around room temperature are monopolized by bismuth telluride ( $\text{Bi}_2\text{Te}_3$ ). However, due to the toxicity and scarcity of tellurium (Te), it is vital to develop a next-generation technology to mitigate the potential bottleneck in raw materials supply for a sustainable future. Hereby, we develop a Te-free n-type compound  $\text{Mg}_3\text{Sb}_{0.6}\text{Bi}_{1.4}$  for near-room-temperature applications. A higher sintering temperature up to 1073 K is found beneficial in reducing the electrical resistivity, but only if the Mg is heavily overcompensated in the initial stoichiometry. The optimizations of processing and doping yield a high average  $zT$  of 1.1 in between 300 K and 573 K. Together with the p-type MgAgSb, we demonstrate module-level conversion efficiencies of 3% and 8.5% under temperature differences of 75 K and 260 K, respectively, and concomitantly a maximum cooling of 72 K when used as a cooler. Besides, the module displays exceptional thermal robustness with a < 10% loss of the output power after thermal cycling for ~32000 times between 323 K and 500 K. These proof-of-principle demonstrations will pave the way for robust, high-performance, and sustainable solid-state power generation and cooling to substitute the highly scarce and toxic  $\text{Bi}_2\text{Te}_3$ .

# Session II

Materials for Sustainable Cooling Applications

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**Prof. Dr. Armin Feldhoff**

## **Thermoelectric cooling - The prospects of calcium cobaltate as p-type component in an efficient entropy pump**



*Prof. Dr. Armin Feldhoff  
Leibniz University Hannover,  
Germany*

Thermoelectric cooling relies on the Peltier effect, which is the electrical induction of a thermal current, in an all-solid-state device without moving parts. A thermoelectric cooler converts electrical energy into directed thermal energy (directed heat), lifting entropy from a low temperature compartment to a higher temperature. It works against the tendency of entropy to flow from a high temperature to a low temperature. By alternately connecting n- and p-semiconductor materials in electrical series and thermally in parallel, such a device can be realized. Currently, thermoelectrics are dominant in small-scale cooling, i.e. below 25 W thermal power, where conventional vapor compression refrigeration systems are not competitive in terms of cost and efficiency. For more than six decades, the technology has been based on bismuth telluride thermoelectric materials, which are evaluated in terms of resource chemistry. Materials that perform better at room temperature are needed to make thermoelectric cooling economically feasible for large-scale cooling systems. The full potential of p-type misfit layered calcium cobaltate has not yet been realized. Its highly anisotropic thermoelectric properties are consistent with the crystal structure, and the anisotropic enhancement by grain alignment in polycrystalline ceramic appears to be the most favorable. Resource chemistry assessment is provided.

# Session II

## Materials for Sustainable Cooling Applications

Dr. Andrey Kovalevsky

### Thermoelectrics for Sustainable Future: The Case of Strontium Titanate



Dr. Andrey Kovalevsky  
University of Aveiro

Thermoelectric technology is pivotal for a sustainable future, providing a solution to one of the most persistent challenges of modern society: energy efficiency. By directly converting heat into electricity (Seebeck effect), thermoelectric generators enable the recovery of energy that would otherwise dissipate uselessly into the environment. They can also offer a cooling capability, utilising the Peltier effect to create a temperature gradient, based on solid-state devices that are compact, reliable, silent in operation and relatively lightweight. This adaptability to both power generation and refrigeration underscores their potential to play a dual role in the green and sustainable energy landscape. Both the energy efficiency of thermoelectric harvesting and coefficient of performance of thermoelectric cooling depend on thermoelectric figure-of-merit,  $ZT = \sigma \alpha^2 T / k$ , where  $\sigma$  and  $k$  are the electrical and thermal conductivities of a thermoelectric material,  $\alpha$  is the Seebeck coefficient or thermopower, and  $T$  is the absolute temperature. The material of choice must exhibit an optimal combination of these fundamental physical properties to maximise the figure of merit ( $ZT$ ) and achieve superior thermoelectric performance [1].

Oxide materials, composed of naturally abundant, non-toxic elements, are recognised as a viable alternative to conventional thermoelectrics. They offer the capability to operate at elevated temperatures, which leads to enhanced Carnot efficiency, and exhibit remarkable structural and microstructural versatility. Strontium titanate ( $\text{SrTiO}_3$ ) emerged as a front-runner among n-type oxide thermoelectrics owing to its promising electronic properties, phase stability, and exceptional flexibility for tuning by substitution and incorporating A-site and oxygen deficiency [2]. In addition, strontium titanate is chemically compatible with many other materials, enabling a variety of thermoelectric composite approaches.

While contemporary  $\text{SrTiO}_3$ -based materials typically exhibit thermoelectric performance with  $ZT$  values reaching 0.4 [3],  $ZT$  values close to or above unity are required for potential applications. Recent studies have evidenced that higher  $ZT$  values can be achieved in  $\text{SrTiO}_3$ -based composites containing graphite [4] and MXene [5] inclusions. Graphene incorporation expands the operational temperature range to include room temperature [6], enabling potential cooling applications. The current cooling performance of  $\text{SrTiO}_3$ -based materials at nearly room temperature is significantly lower than that of traditional thermoelectric materials due, in part, to the mainstream research focus on harvesting intermediate- and high-temperature waste heat. However, for  $\text{SrTiO}_3$ -based thermoelectrics, the inherent high thermal conductivity can be offset by enhancing the power factor, a critical factor for certain cooling scenarios.

Acknowledgements. AK acknowledges the support of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC).

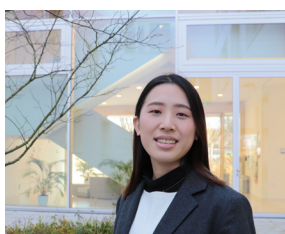


# Session III

Green materials for Green Hydrogen

Chi-Chia Lin

## Enhancing magnetic properties and rare earth element utilization efficiency of Ce-containing Nd-Fe-B magnets by the 2-powder method (Contributed Talk)



Chi-Chia Lin  
Fraunhofer IWKS

Neodymium-iron-boron (Nd-Fe-B)-based permanent magnets are experiencing heightened demand owing to the rapid development of green technologies [1]. This work delves into the realm of cerium-containing (Ce,Nd)-Fe-B magnets presenting an opportunity to alleviate the currently high reliance on critical rare earth elements (REEs) like Nd, Pr, and Dy. Considering the natural abundance, the integration of the most plentiful REE Ce into Nd-Fe-B-based magnets is a promising solution to reduce costs, balance REE demands, and lower environmental impacts. However, the substitution poses challenges to maintaining high magnetic performances due to the intrinsic properties of the  $\text{Ce}_2\text{Fe}_{14}\text{B}$  phase, which are inferior to those of the  $\text{Nd}_2\text{Fe}_{14}\text{B}$  phase [2].

To counteract this deterioration, the 2-powder method (2PM) offers a solution[3,4]. This method involves blending a size-finer powder (AP) exhibiting a higher anisotropy field with a coarser main powder (MP), both possessing a  $\text{RE}_2\text{Fe}_{14}\text{B}$ -based composition. The resulting core-shell structure, achieved by a standard sintering procedure, magnetically hardens the  $\text{RE}_2\text{Fe}_{14}\text{B}$  grain surface, thereby improving coercivity. Advantageously, as the source with a higher anisotropy field is blended homogeneously with MP before sintering, there are no limitations in magnet sizes or shapes. Investigation into Nd-rich and Dy-rich APs of Nd-Fe-B and (Nd,Dy)-Fe-B on the (Ce,Nd)-Fe-B MP reveals that elemental distribution within the core-shell structure significantly impacts magnetic performances. Applying Nd-rich AP leads to a Nd-rich as well as Pr- and Ce-lean shell on  $\text{RE}_2\text{Fe}_{14}\text{B}$  grains, resulting in a 25% improvement in coercivity compared to magnets manufactured solely with MP. Significantly, utilizing Dy-rich AP yields an extraordinary 81% increase in coercivity by including only 3 wt.% of Dy without compromising remanence. This remarkable enhancement is attributed to the tendency of Dy to substitute Ce rather than Nd nor Pr in the  $\text{RE}_2\text{Fe}_{14}\text{B}$  phase. The preference occupancies of different REEs in the shell region of  $\text{RE}_2\text{Fe}_{14}\text{B}$  grains are clues to make the 2PM optimally efficient in REE utilization. In conclusion, the 2PM emerges as a viable strategy with high REE utilization efficiency for improving the magnetic performances of (Ce,Nd)-Fe-B magnets. Through meticulous optimization of RE composition in the MP and AP, magnetic properties can be finely tuned while minimizing reliance on those more critical REEs, helping to maintain environmental sustainability.

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# Session III

Green materials for Green Hydrogen

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**Prof. Dr. Ulrike Kramm**

## How rethinking the chemistry of iron can contribute to a more sustainable future



*Prof. Dr. Ulrike Kramm  
Technische Universität Darmstadt, Germany*

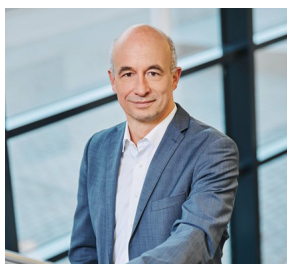
For the energy transition we aim to dispel fossil fuels from our society. In order to enable this, renewable energies are important to fill the related energy gap. In this respect electrochemistry offers several solutions for energy storage and conversion by the use of (super-)capacitors, batteries as well as electrocatalysis in fuel cells and electrolyzers ( $H_2$  and  $CO_2$ ). In several of such devices critical raw materials are used, like platinum in fuel cells and iridium and platinum in hydrogen electrolyzers. If we would like to become sustainable in a general perspective, it is necessary to not only develop sustainable technologies but also using earth abundant elements to replace precious group metal catalysts. In proton exchange fuel cells (PEFCs), iron nitrogen carbon (FeNC) catalysts reach similar activities but still need to be improved in terms of durability in comparison to platinum.[1] From its chemistry iron by itself would not be stable under PEFC operation. However, induced by nitrogen ligands, the iron is stabilized making it applicable even in PEFCs. This illustrates the importance of the local environment on the reactivity of iron.[2-5] In our CRC Iron, upgraded! we use this approach and explore systematically,[6] how the local environment changes the properties associated with iron aiming for structure-property maps for different fields of application and to deduce general trends in chemistry. In this work, I will introduce the concept of our CRC towards a sustainable materials database and highlight some of the results for the FeNC catalysts.

# Session III

Green materials for Green Hydrogen

Dr. Steffen Hasenzahl

## Successful development and scale-up of materials as pre-condition for a climate-neutral hydrogen economy



Dr. Steffen Hasenzahl  
Evonik Operations GmbH  
Creavis

Successful development and scale-up of materials as pre-condition for a climate-neutral hydrogen economy

The world is on its way to a net-zero society, and the availability of climate-neutral hydrogen is a key factor in the success of the energy transition. Not only the chemical industry, but also other sectors such as the steel industry or the mobility sector will require large quantities of hydrogen that is produced without carbon dioxide emissions.

The one preferred route to climate-neutral hydrogen is based on water electrolysis using renewable electricity (so-called green hydrogen). Three low-temperature water electrolysis technologies are available today. The most mature technology is alkaline electrolysis (AEL) with a diaphragm as a separator between the two half-cells in which hydrogen and oxygen are formed. Less mature is PEM electrolysis (proton exchange membrane), followed by AEM electrolysis (anion exchange membrane), both of which use an ion exchange membrane as a separator. AEM technology has the potential to enable the most cost-effective green hydrogen production as it combines the advantages of AEL and PEM electrolysis without their drawbacks. Similar to AEL, the alkaline medium enables the use of low-cost electrocatalysts and electrolyzer components. Like PEM electrolysis, the polymer membrane enables operation at high current densities and hydrogen production under differential pressure. To realize these advantages, the anion exchange membrane must combine high ion conductivity with excellent chemical and mechanical stability. Most existing anion-conducting membranes are deficient in at least one of these critical performance parameters.

Here we report on the development of an anion-conducting polymer and its use for producing the novel DURAION® anion exchange membrane. It will be shown, how extensive screening of various monomers and detailed laboratory-scale testing of the ion-conducting polymers formed led to the identification of a system that combines the key properties described above. In addition, the scale-up of monomer and polymer synthesis as well as the scale-up of membrane production from hand-casting to small-scale, continuous roll-to-roll production will be presented. In order to ensure consistent quality of the membranes produced, various analytical methods had to be developed. Among others, hydrogen cross-over, ionic conductivity and electrolysis performance tests will be discussed. Finally, we will discuss the latest developments in terms of high performance electrocatalysts for anion exchange membrane AEM electrolysis, both on the HER (hydrogen evolution reaction) and OER (oxygen evolution reaction) side.

# Session III

Green materials for Green Hydrogen

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Dr. Thomas Fischer

## On the Way to Sustainable Hydrogen: Visions and Limitations of Photoelectrochemical Water Splitting Technologies



*Dr. Thomas Fischer*  
*University of Cologne*

Hydrogen is widely discussed as the prime future energy carrier in terms of gravimetric energy density and availability through water splitting, but inherent limitations in efficient storage and transportation capabilities limit a widespread technology rollout. Moreover, green alternatives for hydrogen production apart from electrolysis based on renewable energies must be established to diversify the production landscape for increased security of supply and decentralized logistics. Apart from thermochemical cycles and biological hydrogen production direct conversion of solar energy to chemical energy in photochemical or photoelectrochemical systems are discussed as viable and scalable technologies. Efficient photocatalysts providing high photocurrents at low overpotentials with inherent stability combined with raw material availability are of key importance to establish this technology as a feasible addition in the growing hydrogen economy. The presentation will review current advances in the development of catalysts for photoelectrochemical water splitting reactions and highlight the technological potential as well as limitations in terms of scalability and resource demands.

# Session III

Green materials for Green Hydrogen

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**Andreas Brumby**

## **Critical Raw Materials for the Hydrogen Economy**



*Andreas Brumby  
Materials Valley e.V.*

The EU Commission proposed in March 2023 the ECRMA (European Critical Raw Materials Act). Andreas will give a short introduction on the ECRMA and discusses the implications especially for the emerging Hydrogen Economy, e.g. for electrolysis development. He will also mention the PFAS (Per- and polyfluoroalkyl substances) legislation process and by this stressing the necessity of »supply chain thinking«.

# Session III

Green materials for Green Hydrogen

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Prof. Dr. Ümit Demirci

## BN(C)H materials for hydrogen storage and production



*Prof. Dr. Ümit Demirci  
European Institute for Mem-  
branes and  
University Montpellier*

Ammonia borane (AB) has a rich history in the realm of chemical hydrogen storage. Discovered in the mid-20th century, it was re-discovered in the early 21st century and has been extensively studied in the past two decades. AB naturally stores 19.5 wt% of hydrogen and can release >67% of it when heated to 200 °C. This release can occur below 100 °C when AB is destabilized, for example, through nanoconfinement.

AB has also paved the way for various BN(C)H compounds, often derived from it. Examples of these derivatives include metal amidoboranes, hydrazine borane, alkylamine boranes, as well as boron nitride (pure or carbon-doped) and borocarbonitride. Remarkably, all of these compounds have, at one point or another, been considered for chemical or physical hydrogen storage.

In our group, we have explored these derivatives. Initially, our focus was on their role as hydrogen carriers, particularly in the case of hydrides. Subsequently, we investigated their potential for physical hydrogen storage, emphasizing boron nitride-based porous systems. Recently, we have observed that some exhibit the potential to capture gases beyond hydrogen, sparking new interests in gas capture, hydrogen separation/purification. The upcoming ICRC 2024 meeting will provide an excellent opportunity to showcase our latest achievements.

# Session III

## Green materials for Green Hydrogen

### Nikita Gugin

## Large-Scale Green Synthesis of a Model BSA@ZIF-8 Biocomposite via Reactive Extrusion (Contributed Talk)



Nikita Gugin  
Bundesanstalt für Materialforschung und -prüfung (BAM)

Metal-organic framework-based biocomposites (MOF-biocomposites) hold significant promise for applications in biosensing, biocatalysis, and delivery of biopharmaceuticals.[1] One of the most studied MOFs for bioapplications is ZIF-8 (zeolitic imidazolate framework 8) due to its high surface area, high thermal and chemical stability, and low cytotoxicity.[2] The conventional synthesis method for ZIF-8-biocomposites, known as biomimetic mineralization, involves mixing specific biomolecules, 2-methylimidazole, and a soluble  $Zn^{2+}$  source in water.[3] While this method is highly efficient, it has limitations in terms of scalability and is restricted to hydrophilic biomolecules. Aimed at developing a scalable and versatile approach, we adapted our recently reported ZIF-8 reactive extrusion[4] for biocomposite production.

For the preparation of biocomposites, bovine serum albumin (BSA) was selected as an inexpensive model biomacromolecule. The synthesis of BSA@ZIF-8 was carried out using a twin-screw extruder at a mild temperature of 40 °C, employing a catalytic amount of EtOH following our previously explored procedure[4]. Comprehensive characterization using powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA), FTIR,  $N_2$  adsorption, confocal laser scanning microscopy (CLSM), and Bradford assay allowed us to optimize reaction conditions and quantify the amount of encapsulated BSA.

After thoroughly washing the extrudate with ethanol to eliminate surface-adsorbed BSA molecules, we obtained highly crystalline and pure BSA@ZIF-8 with varying BSA loadings. Notably, achieving a maximum BSA encapsulation of 26wt% was possible with 40wt% BSA in the reagent mixture. With 5wt% BSA, we reached a high encapsulation efficiency of 96%, a critical aspect for the cost-effective production of biocomposites involving expensive biomolecules. A continuous extruder operation under optimized conditions demonstrated consistent product quality, enabling the production of biocomposites on a 1.2  $kd\ d^{-1}$  scale with a space-time yield of approximately 30000  $kg\ m^{-3}\ d^{-1}$ . These findings offer valuable insights into the cost-effective and large-scale production of ZIF-8-based biocomposites. Moreover, due to its solid-state nature, this reaction is independent of the hydrophilic or hydrophobic properties of biomolecules, providing flexibility and advantages over solvent-based processes.

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# Session III

Green materials for Green Hydrogen

Dr. Andreas Hertwig

## New analytic ways to characterise mesoporous



*Dr. Andreas Hertwig  
Bundesanstalt für Materialfor-  
schung und -prüfung (BAM)*

Mesoporous materials are needed in many applications where a high specific surface area and adsorptive in Mesoporous materials are needed in many applications where a high specific surface area and adsorptive behaviour is needed. Important examples are separation techniques and barrier layers and catalysts. Electrochemical water splitting is the key technology for producing green hydrogen and there is no foreseeable alternative to this process for producing elementary hydrogen from green electrical power. Water electrolysis can be divided into the anodic Oxygen Evolution Reaction (OER) and the cathodic Hydrogen Evolution Reaction (HER). Both processes have to be heavily optimised to a large extent to avoid energy losses caused by overvoltage. The development of electrodes for these processes is especially difficult due to the many boundary conditions. Water splitting is a catalytic as well as electrochemical process. The contact area between the electrolyte and the electrode must be maximised maintaining the stability of the surface. Side reactions must be suppressed, and effective gas transport must be ensured. The whole process has to be tolerant with respect to temperature, harsh chemical conditions from the electrolyte as well as high current densities.

We present a hybrid analytical method combining several analytical techniques for determining the properties of thin layers of mixed oxides of the general composition Ir:TiO<sub>x</sub>. These materials are promising candidates for electrocatalytic top coatings of OER electrodes. To lower the costs of the electrolyzers, the main goal is to lower the Ir content retaining the system efficiency. The main properties which are hard to determine are the porous volume fraction and the Ir:Ti element ratio. By a combination of electron microscopy, spectroscopic operando ellipsometry, ellipsometric porosimetry, and other techniques, we can determine key features of mesoporous thin layer materials. We aim to develop operando capable techniques used in process monitoring as well as measurement techniques optimised for accuracy. By developing reference materials, we support long term uptake of our methodology. This work can directly be used for optimising electrocatalytic layers and is a good example for the power of hybrid metrology for improving materials design. electrocatalytic water splitting.



# Session IV

Green Batteries

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**Dr. Guinevere Giffin**

## **Sustainable Battery Production as a Design for Recycling Concept**



*Dr. Guinevere Giffin  
Fraunhofer Institute for Silicate Research ISC*

Awareness of the importance of sustainability and environmental impacts in the battery sector is increasing following decades of focus almost solely on improving performance of batteries. The need for sustainability is present along the full value chain, from resources to cell production and recycling. This contribution addresses sustainable battery production in the context of a design for recycling concept supporting direct recycling. In particular, the contribution of the Fraunhofer Research and Development Center for Electromobility (FZEB) at the Fraunhofer Institute for Silicate Research ISC will be highlighted.

# Session IV

## Green Batteries

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### Prof. Emma Kendrick

## Designing sustainability into new battery chemistries



*Prof. Emma Kendrick*  
*University of Birmingham*

To create better and more sustainable battery chemistries, it is important to consider all aspects of the battery cycle. This includes factors such as raw materials and their supply chain, manufacturing processes of materials, electrodes and cells, performance properties, and recycling or end-of-life processes. This presentation will discuss the importance of both critical and non-critical materials in batteries and their use in different battery chemistries. Lithium-ion batteries often contain high value elements such as cobalt or nickel which means that the current recycling processes are more viable, however for lower value materials such as lithium iron phosphate or the sodium-ion cathode materials lower cost recovery processes are required. If the materials can be recovered easily with low-cost processes routes and in a form that can be directly re-used in a battery, direct recycling, the economics should be more favourable than returning to the elements to either their metallic or precursor salt as is done in pyrometallurgical and hydrometallurgical routes. When developing new battery technologies, there's a chance to design in recycling from the start, rather than retrospectively, as is currently the case for lithium-ion batteries. Additionally, this presentation will explore design principles for creating a more sustainable battery technology.

# Session IV

## Green Batteries

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Dr.-Ing. Magdalena Graczyk-Zajac

### Towards sustainable, grid connected stationary storage system: ResHy project



*Dr.-Ing. Magdalena  
Graczyk-Zajac  
TU Darmstadt and  
EnBW Energie Baden-Würt-  
temberg AG*

Generation and load peaks from renewable energy sources are a challenge for energy grids. There is no single energy storage solution that is ideal for every grid-scale application. Combining storage components into a complex system allows to benefit on the advantage and to suppress weak points of the components. Hybrid energy storage systems (HESS) refer to several types of storage components of different characteristics that are combined to form an integral entity, preferably controlled by a mutual energy management system.

Usually, an electrochemical energy storage system is designed either for high-power or high-energy applications and if not used in intended ways, the user must cope with penalties by lifetime, performance, and cost. In this talk, an example of a flexible and sustainable storage system which is being developed within ResHy\* project by EnBW AG and Fraunhofer ISE will be presented. ResHy aims the development of an electrochemical hybrid storage system containing a 2nd life lithium-ion battery (LiB) and a sodium-based component. To improve the efficiency and benefit on synergies of the single components, an energy management system (EMS) and a highly flexible control system will be developed. This will allow a high degree of control and adaptability, as well as better adjustment to a variety of system environments. The developed hybrid storage system will be implemented and tested at a solar park of 62 MWp planned by EnBW in Gundelsheim, proximity of the city Heilbronn.

\*ResHy: Ressourcenschonende Hybridbatterie – Bau, Integration und Betriebsoptimierung,  
English: Sustainable hybrid battery - design, integration and performance optimization

# Session IV

## Green Batteries

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**Prof. Dr. Monika Wilamowska-Zawłocka**

### **Challenges of direct recycling of used lithium-ion batteries**



*Prof. Dr. Monika  
Wilamowska-Zawłocka  
Gdańsk University of  
Technology*

Various recycling methods for lithium-ion batteries (LIBs) have already reached the industrial stage. However, there is a significant need to improve these processes towards greater sustainability. Currently, commercial recycling of LIBs mainly focuses on recovering precious metals, particularly cobalt, copper, and nickel. Recovery of other valuable elements and components, such as lithium or graphite, is still limited to laboratory scale. Direct recycling is a method that recovers active materials while preserving their original structure. The direct recycling approach offers significant advantages, including lower emissions and less secondary pollution compared to pyrometallurgical and hydrometallurgical processes. However, there are many challenges to overcome to make direct recycling viable. In this work, we explore various aspects and problems of direct recovery of graphitic anodes and lithium-nickel-manganese-cobalt-oxide (NMC) cathodes. One challenge is separating electrode layers from current collectors, as they are designed to have long-lasting adhesion. Polyvinylidene fluoride (PVDF) binder, widely used in commercial batteries, exhibits strong binding forces and is problematic to remove in a sustainable way. Here we present several ways of: i) separation of electrode layers from current collectors, ii) removal of PVDF binder and iii) recovery of active materials. The methods differ depending on anode or cathode side. The achieved capacity values for the recovered NMC 532 cathode and graphitic anode reaches 140 and 370 mAh g<sup>-1</sup>, respectively, after 100 charge-discharge cycles at C/10 current rate (charging in 10 hours).

#### Acknowledgements

Financial support from SONATA-BIS program of the National Science Centre, Poland, project "Development of processes for critical raw materials recovery from spent lithium-ion cells", grant no. UMO-2022/46/E/ST8/00395 is gratefully acknowledged.

# Session IV

## Green Batteries

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### Dr. Songhak Yoon

## How to revitalize the spent lithium-ion batteries



*Dr. Songhak Yoon*  
*Fraunhofer IWKS*

Although the benefits of recycling spent lithium-ion batteries (LIBs) are widely acknowledged, many challenges and issues persist. Spent LIBs are expected to be collected, sorted, dismantled, and finally converted into black mass (BM). This is the so-called pre-treatment in recycling processes. While BM producing and processing technologies have been gaining momentum in recent years, the BM market is still in its infancy and requires for improvements in terms of economic feasibility and environmental footprint. Moreover, relevant regulatory frameworks need to be updated concerning the widespread use and advancement of LIBs. The technical challenges lie in the post-treatment during leaching of BM and precipitation of the valuable metals to revive the spent LIBs. BM is typically dissolved in an acidic or alkaline solution and followed by selective but complex extraction of valuable metal compounds. Various complex separation processes are necessary in the post-process phase to bring BM back into the battery production. In the post-treatment, two main challenges are increasingly apparent nowadays due to political and/or economic circumstances. One is the significant investment required for building the infrastructure. The other one is creating sustainable cycles and finding the pathways to the decarbonized recycling processes, while embracing the challenges of tomorrow. Thus, a holistic view of the current recycling process is vital to minimize negative effects on the environment. As an alternative to the current hydrometallurgy, direct recycling has emerged but commercialization of those lab-scale processes still needs to be validated from industrial perspectives. Finding solutions for these challenges in the end requires efforts not only from the scientists and researchers, but also from industrial stakeholders with growing interests and long-term patient engagement for the technical breakthrough. However, this is understandably very difficult as making a profit is an essential component of a successful business. Due to declining profitability and income, the LIB recycling industry is facing an increasingly severe struggle for survival. In this regard, battery regulations and legal supports are eagerly anticipated for the industries to keep high levels of commitments to long-term investments. Moreover, it is urgent to strengthen the competitiveness by closely monitoring geopolitical policy movements mainly in China, U.S.A., and Europe by deepening cooperation with local and overseas companies and governments. In this contribution, current achievements and remaining challenges in LIB recycling carried out in Fraunhofer IWKS will be presented. Our exploration of alternative hydrometallurgical processes using deep eutectic solvents (DES) will be covered. Finally, the advancements and challenges for sustainable BM recovery will be discussed.

# Session V

Plasma-assisted CO<sub>2</sub> (&H<sub>2</sub>) Utilization

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Prof. Dr. Xin Tu

## Plasma catalysis: A promising solution for decentralized production of fuels and chemicals



*Prof. Dr. Xin Tu*  
*University of Liverpool*

The conversion of inert molecules (e.g., CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>) with strong chemical bonds for the synthesis of value-added synthetic fuels and platform chemicals has attracted significant interest. However, the activation of these molecules remains a great challenge due to their thermodynamical stable, requiring a substantial amount of energy for activation. Non-thermal plasma (NTP) has emerged as a promising technology for gas conversions under ambient conditions. The combination of NTP with heterogeneous catalysis has great potential for achieving a synergistic effect through the interactions between the plasma and catalysts, which can activate catalysts at low temperatures, improve their activity and stability, and lead to a notable increase in conversion, selectivity, and yield of end-products, as well as enhance the energy efficiency of the process. Furthermore, plasma processes can be switched on and off instantly, offering great flexibility in decentralised fuel and chemical production using renewable energy sources, particularly intermittent renewable energy. This presentation will discuss the opportunities and challenges in plasma-catalytic gas conversion to fuels and chemicals, including various chemical processes such as CH<sub>4</sub> activation, CO<sub>2</sub> conversion, and ammonia synthesis.

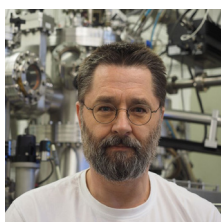
# Session V

Plasma-assisted CO<sub>2</sub> (&H<sub>2</sub>) Utilization

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**Dr.-Ing. Andreas Schulz**

## Activation of low-energy molecules using the example of CO<sub>2</sub> in microwave air plasmas



The chemical industry faces the challenge of defossilization to counteract climate change. One way to produce basic chemicals from renewable resources is to activate inert molecules such as CO<sub>2</sub>, H<sub>2</sub>O or N<sub>2</sub>. A microwave plasma process is presented to activate CO<sub>2</sub> and provide CO as a base chemical.

*Dr.-Ing. Andreas Schulz*  
*University of Stuttgart*

# Session V

Plasma-assisted CO<sub>2</sub> (&H<sub>2</sub>) Utilization

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**Dr. Amandine Guissart**

## Microwave plasma sources for sustainable applications



*Dr. Amandine Guissart*  
*Muegge GmbH*

Microwave plasma sources are designed to generate a contact-free plasma while ensuring stable operation for a wide parameter range of gas-types, gas flow and microwave power at 2.45 GHz and 915 MHz. These plasma sources are well suited for both, the synthesis of special gases and for supporting chemical reactions with highly reactive gas species. This is the key for a wide range of industrial applications. Power-to-X applications such as Power-to-Gas and Power-to-Chemicals are prominent examples of industrial applications based on these microwave plasma sources. The contactless plasma generation is the key property of these microwave energy driven high temperature applications. Moreover, microwave plasma systems offer the best alternative to build decentralized supply networks with CO<sub>2</sub>-neutral hydrogen-based fuel gases. Such gases can in turn be employed for energy storage or for direct and location-independent use. Power-to-X technologies based on microwave plasma processes are then innovative solutions to convert surplus electrical energy from renewable sources into material resources such as hydrogen, carbon monoxide, and synthetic gases for storage and recycling, e.g., conversion of electrical energy into gaseous or liquid fuels or chemicals for long-haul trucking, shipping and aviation. This contribution reviews some of these applications.



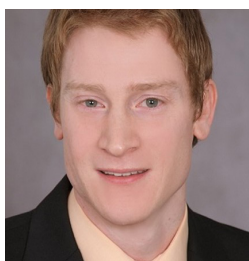
# Session V

Plasma-assisted CO<sub>2</sub> (&H<sub>2</sub>) Utilization

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Dr. Marc Widenmeyer

## Merging Materials Performance and Sustainability: Ceramic Oxygen Transport Membrane Materials as an Exemplar



*Dr. Marc Widenmeyer  
Technical University of Darmstadt, Research Group Materials & Resources*

Human activities have already surpassed six of the nine quantified planetary boundaries. Our current performance-orientated material development patterns and technological advancements within a linear value chain continuously contribute to it by a steadily increasing resource demand, greenhouse gas emissions, and accruing waste, despite growing awareness. For a sustainable future, we need to change production and use of materials by implementing a circular economy. In that context, we are investigating ceramic oxygen transport membrane materials (OTM) as an enabler of microwave plasma-based CO<sub>2</sub> and green H<sub>2</sub> utilization. The OTM are needed to control the oxygen partial pressure in the reaction zone helping to suppress side reactions; thereby, enhancing product efficiency. The application in a plasma environment puts a high demand on the selected material. Additionally, the material needs to be recyclable and bear low environmental impacts (EIs) to align with the European Commission's new circular economy action plan. We are implementing several pathways towards well-performing sustainable OTM: i) using classical and very recent materials science tools such as Ellingham diagrams and Fermi Level Engineering, respectively, to improve the separation performance, ii) replacing as much as possible critical elements without agitating functionality, and iii) implementing (chemical) recycling at the early-stage of materials development. All these measures are simultaneously accompanied by screening life cycle assessments to identify the major contributors to the EIs, hence establishing a roadmap for sustainability improvements solely based on robust scientific data. In summary, the presented case studies demonstrate the importance of performing a sustainability assessment during the early stages of materials or process development to genuinely progress towards a sustainable future. This recommendation is broadly applicable, while the specific results of the case studies should be only generalized or extrapolated with utmost care.

# Session V

## Plasma-assisted CO<sub>2</sub> (&H<sub>2</sub>) Utilization

Dr. Thomas Schiestel

### Hollow fiber and membrane module fabrication



*Dr. Thomas Schiestel  
Fraunhofer Institute for  
Interfacial Engineering and  
Biotechnology*

One of the biggest challenges for the next decades is to stop the process of global warming. A possible approach to decrease the CO<sub>2</sub>-emission could be the use of CO<sub>2</sub> in power-to-X applications. Here, we present the use of MIEC hollow fiber membranes in a so-called plasma-membrane reactor to separate oxygen from a CO<sub>2</sub> plasma. In the plasma, the CO<sub>2</sub> is splitted into oxygen and CO, which can be used as a platform chemical for further syntheses (e.g. Fischer-Tropsch). Experimental. In the project, hollow fiber membranes from various MIEC materials (e.g. (La<sub>0.6</sub>Ca<sub>0.4</sub>)(Co<sub>0.8</sub>Fe<sub>0.2</sub>)O<sub>3- $\delta$</sub>  (LCCF)) were manufactured using a wet spinning process. Subsequently, the hollow fibers were sintered to receive gastight membranes with an outer diameter of 1.2 mm. The sintered membranes were further treated by an etching process to increase the active surface of the membranes. The oxygen permeation of the LCCF hollow fibers were tested both in a normal furnace and in a microwave induced atmospheric plasma torch under a CO<sub>2</sub> atmosphere. Results and discussion. Due to the operation in a CO<sub>2</sub> plasma, we are especially interested in the behaviour of the hollow fiber membranes under CO<sub>2</sub> containing atmospheres. Measurements with the hollow fibers in the furnace reveal both a good stability in a gas composition with 50 % CO<sub>2</sub> and a high oxygen permeation. Thereby the permeation depends strongly on sintering condition [1] and surface treatment and oxygen permeation of up to 5.1 ml min<sup>-1</sup> cm<sup>-2</sup> at 1000°C can be achieved [2]. In the CO<sub>2</sub> plasma the capillaries are repeatedly heated up to temperatures above 1000°C within seconds without any damage and no degradation could be observed even after long time treatment. Measurements with the CO<sub>2</sub>-stable LCCF hollow fibers in the plasma verify the splitting of CO<sub>2</sub> into CO and O<sub>2</sub>. In the plasma-membrane reactor, an oxygen permeation up to 1,5 ml min<sup>-1</sup> cm<sup>-2</sup> was achieved. It was possible to perform O<sub>2</sub> separation from the CO<sub>2</sub> plasma with modules with up to 27 fibers [3]. Accordingly, a plasma coupled membrane reactor is a reasonable option to separate oxygen and prevent the back reaction of CO<sub>2</sub> to generate CO.

#### Acknowledgments

We gratefully acknowledge the support of the German Federal Ministry of Education and Research (grant number 03SF0618C).

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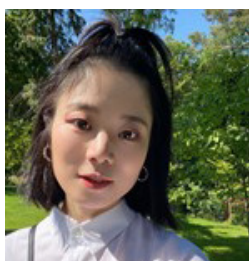
# Session VI

## Chemical Recycling of Plastics

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Dr. Yeshui Zhang

### Advanced Metrology for Studying Catalyst Degradation & Li-ion Battery Drying Process



Dr. Yeshui Zhang  
University of Aberdeen

Insightfully understanding the process of volatiles from plastic depolymerization entering from the exterior into internal structure of catalyst favors to rationalize the catalyst design in scale-up principles. Herein, catalytic degradation of plastic wastes with fluid catalytic cracking catalyst (FCC) was investigated in-depth. The structural evolution of catalyst on overall scope, including the topology of heterogeneous pore systems and spatial distribution of zeolite was probed by X-ray nano-CT. The results showed that FCC enhanced the transformation of C16-C30 chains to C9-centered monocyclic aromatics. The nano-CT analysis of FCCs illustrated remarkable loss of exterior porosity after reaction, particularly at the depth of  $\sim 16.5 \mu\text{m}$  from the outmost layer. While the interior pores were marginally affected, indicating large hydrocarbons incapable of engaging with active sites to full advantage, which preferably occupied large-size pores ( $>385 \text{ nm}$ ) of external surface. The performance of Li-ion batteries is determined by the architecture and properties of electrodes formed during manufacturing, particularly in the drying process when solvent is removed and the electrode structure is formed. A comparison of temperature effects on both NMC622-based cathodes (PVDF-based binder) and graphite-based anodes (water-based binder) dried at RT, 60, 80, 100 and 120 °C has been undertaken. X-ray computed tomography showed that NMC622 particles concentrated at the surface of the cathode coating except when dried at 60 °C. However, anodes showed similar graphite distributions at all temperatures. Focused-ion beam scanning electrode microscopy and energy-dispersive X-ray spectroscopy suggested that the F-rich binder distribution was largely insensitive to temperature for cathodes. To date there is limited discussion of these processes in the literature due to the limitation of existing in-situ metrology. Here, ultrasound acoustic measurements are demonstrated as a promising tool to monitor the physical evolution of the electrode coating in-situ. A possible application of using this technique is to adjust the drying rates based upon the ultrasound readings at different drying stages to speed up the drying time. These findings prove this measurement can be used as a cost-effective and simple tool to provide characteristic diagnostics of the electrode, which can be applied in large scale coating manufacturing.

# Session VI

## Chemical Recycling of Plastics

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### Prof. Dr. Holger Helten

## Furan-based optoelectronic materials from renewable resources – a successful example where sustainability and performance go hand in hand



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Würzburg (JMU), Institute of  
Inorganic Chemistry and Insti-  
tute for Sustainable Chemistry  
& Catalysis with Boron (ICB)*

Materials used as the active layers of organic optoelectronic devices such as organic LEDs and organic solar cells are almost exclusively based on petrochemical starting materials. Their production still relies on relatively energy-intensive processes and often uses hazardous and environmentally harmful reagents. Efforts aimed at the development of recyclable materials for these purposes are scarce. Furan derivatives can be obtained from the platform chemical furfural and thus are derived from lignocellulosic biomass. Furan rings are also biodegradable. For optoelectronic applications, furan-based materials offer several advantageous features such as exceptionally bright luminescence, good solubility, and effective pi-electron delocalization along their backbone. The reason why they have received relatively little consideration for such applications in the past is their moderate oxidative stability in air, especially in the presence of incident light. Herein, it is demonstrated that furan-containing optoelectronic materials are effectively stabilized through the combination with electron-deficient trivalent boron. In addition, this provides the materials with special features enabling their use for certain sensory applications and as stimuli-responsive materials. Innovative synthetic concepts will also be presented. Our group has developed an environmentally benign organocatalytic polymerization method, which avoids the use of toxic reagents such as organotin compounds previously used in organoboron chemistry.

# Session VI

## Chemical Recycling of Plastics

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**Prof. Dr.-Ing. Martin Gräbner**

### **Overview on thermo-chemical Conversion Processes for Chemical Recycling**



The presentation will place chemical recycling in the existing waste hierarchy and reflect the recent discussion on the topic in the European context. It provides an overview of the different technological options and focuses on the pyrolytic conversion and gasification processes for mixed plastic waste. The general process principles, products and process conditions will be discussed and recent development directions will be analysed and typical concepts will be presented. A market overview of technologies, plant sizes, announced projects and partnerships will be complemented by examples of current commercial implementation and research activities.

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Institute of Energy Process  
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Freiberg, Fraunhofer Institute  
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Systems IKTS*

# Session VI

## Chemical Recycling of Plastics

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Prof. Dr. René Wilhelm

## Chemical Recycling of Carbon Fiber Composites



*Prof. Dr.-Ing. René Wilhelm  
Clausthal University of  
Technology*

The pressing need for effective recycling strategies within the wind energy industry has motivated us to investigate the behavior of various solvents and catalysts used in the solvolysis of carbon fiber reinforced plastics. Our research has revealed that methanesulfonic acid presents itself as an intriguing alternative to conventional solvents and catalytic Bronsted and Lewis acids. In our study, we applied two layers of carbon fibers (CFs) that were impregnated with amine-based epoxy using a vacuum-assisted resin infusion (VARI) process. The findings unequivocally demonstrated that methanesulfonic acid (MSA) stands as the most efficient catalytic solvent for the solvolysis of carbon fiber reinforced plastics (CFRPs), outperforming other commonly investigated acids. Furthermore, the recycled products exhibited commendable properties for both the matrix and the fiber, aligning comparably with virgin materials.

# Session VI

## Chemical Recycling of Plastics

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Prof. Dr. Bert Weckhuysen

### Challenges, Opportunities and Some Mechanistic Understanding in the Chemical Recycling of Plastic Waste



*Prof. Dr. Bert Weckhuysen  
Utrecht University*

Increasing the amount of recycled plastic in our current manufacturing processes of polymer materials, such as polypropylene (PP) and polyethylene (PE), requires the exploration of new methods of chemical recycling of plastic waste. In this lecture, I will discuss three different chemical routes, namely the catalytic pyrolysis, chemical oxidation, and photo-oxidation-solvolysis chemistry of polyolefins.

The first system of interest is the so-called fluid catalytic cracking (FCC) system, which currently converts crude oil fractions into transportation fuels, such as gasoline, and chemical building blocks, such as propylene. We have explored in the past years the use of various FCC systems, containing for example various metal ions, for the catalytic conversion of polypropylene into aromatics. It was found that not only acidity and metal content are of importance, but also the accessibility thereby showing that the overall performance of catalyst materials is determined by the unique balance between active sites and the accessibility or wetting of these active sites. Various spectroscopy and microscopy techniques have revealed the different chemical species involved in the reaction and deactivation mechanism of the catalytic pyrolysis of polypropylene and polyethylene, thereby comparing FCC materials with zeolites and mesoporous materials.

Another system of interest is the oxidation of polyethylene into dicarboxylic acids, thereby comparing the effect of the type of oxidant, namely NO and O<sub>2</sub>. It was found that mixtures of dicarboxylic acids could be formed, which subsequently can be transformed into polyamides in the presence of amines. The addition of transition metal oxides and its effect on the catalytic performance will also be explored.

A third system of interest is the photo-oxidation of plastic waste, in particular low-density polyethylene, thereby combining photocatalysis by a.o. titania with solvolysis. The result of this research is the formation of carboxylic acids, and other oxidation products, such as carbon dioxide, next to microplastics.

The lecture ends with some reflections on the different possibilities of chemical and catalytic technologies to turn plastic waste into valuable products.

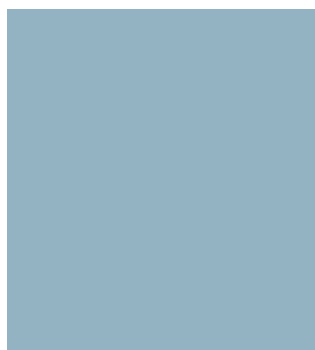
# Session VI

## Chemical Recycling of Plastics

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Tomislav Stolnar

### Upcycling waste PET bottles to porous UiO-66 by mechanochemistry (Contributed Talk)



Tomislav Stolnar  
Bundesanstalt für Materialforschung und -prüfung (BAM)

Single-use plastics are causing plastic pollution, and less than 10% of plastic waste gets recycled globally. Most of it ends up in landfills or gets incinerated in a highly unsustainable manner. Here, I will present a sustainable mechanochemical protocol for the chemical upcycling of polyethylene terephthalate (PET) to porous UiO-66 metal-organic framework (MOF). In the first step, PET is ball-milled with sodium hydroxide and undergoes alkaline hydrolysis to disodium terephthalate ( $\text{Na}_2\text{TP}$ ). Time-resolved in situ monitoring of ball milling reaction by synchrotron powder X-ray diffraction shows the appearance of crystalline  $\text{Na}_2\text{TP}$  after 20 min of milling. However, ex-situ analysis at different milling times by gel permeation chromatography reveals that the depolymerisation step needs more milling for completion. After two hours of ball milling, there are only trace amounts of leftover PET. For upcycling to UiO-66, a zirconium acetate cluster is added to  $\text{Na}_2\text{TP}$  together with liquid additives and after milling for 90 min, results in UiO-66 ( $\text{Na}_2\text{TP}$ ). Alternatively, terephthalic acid (TPA) can be extracted from  $\text{Na}_2\text{TP}$  and ball-milled with zirconium acetate cluster and liquid additives to yield UiO-66 (TPA). We systematically investigated these two distinct synthetic routes and compared their green chemistry metrics, and the crystallinity and gas adsorption properties of UiO-66 ( $\text{Na}_2\text{TP}$ ) and UiO-66 (TPA) materials. UiO-66 ( $\text{Na}_2\text{TP}$ ) route exhibits more favourable green chemistry metrics, but UiO-66 ( $\text{Na}_2\text{TP}$ ) material results in slightly lower crystallinity and BET surface area than UiO-66 (TPA) material. Our results show the potential of mechanochemistry for the sustainable production of high-quality value-added materials such as UiO-66 from waste PET bottles.

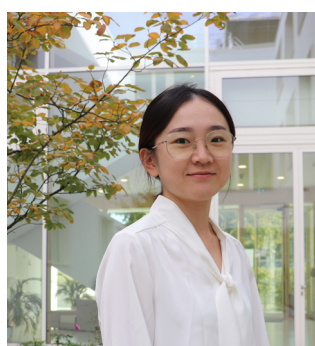


# Session VI

## Chemical Recycling of Plastics

Xiao Yu

### Chemical recycling of medical plastic waste over perovskite-type catalysts for hydrogen production (Contributed Talk)



Xiao Yu  
Fraunhofer IWKS

The growing demand for plastic products in our daily lives generates massive amounts of wastes each year. Further enhanced by the COVID-19 pandemic, the use of single-use medical plastic materials (such as masks and gloves) for health protection has resulted in a significant increase in (micro)plastic post-consumer wastes. The current disposal routes are mainly thermal utilization (incineration) and landfill, which is environmentally unfriendly. More efficient and sustainable recycling methods are desperately needed to turn the waste plastics into value-added chemicals or materials. Chemical recycling approaches like pyrolysis provide a potential cyclic economy route to manage the plastic wastes. The plastic wastes can be directly transformed into chemical products including H<sub>2</sub>-rich gases, hydrocarbon fuels, and carbon nanomaterials.

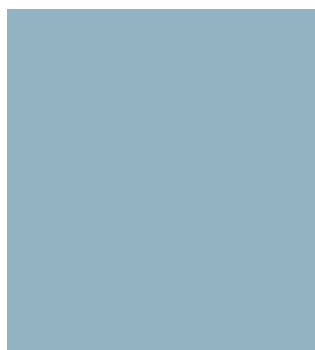
In this work, waste medical masks collected from daily life usage were pyrolyzed and catalytically decomposed with perovskite-type La<sub>0.6</sub>Ca<sub>0.4</sub>Co<sub>1-x</sub>Fe<sub>x</sub>O<sub>3-d</sub> pre-catalysts for co-production of H<sub>2</sub> and carbon composite materials. The influences of catalysis reaction temperature and Co/Fe ratio in the investigated pre-catalysts on the yields and selectivity of the gaseous products and carbon deposition were systematically studied. The physicochemical characteristics of the produced carbon nanomaterials were comprehensively characterized by the state-of-the-art techniques. La<sub>0.6</sub>Ca<sub>0.4</sub>Co<sub>0.2</sub>Fe<sub>0.8</sub>O<sub>3-d</sub> possessed the highest hydrogen and carbon nanomaterials yields at 850 °C among all the investigated pre-catalysts. Especially, this pre-catalyst showed an excellent performance during 10 cycles of successive deconstruction of plastic wastes with the highest hydrogen yield at the 7th cycle. More importantly, carbon nanotubes generated had higher graphitic characteristics and fewer defects. The presented results demonstrated that the developed perovskite pre-catalyst is a promising candidate for co-producing hydrogen and carbon nanotube composites for energy storage applications from medical waste plastics.

# Poster Sessions

P01

Yoko Matsuzawa

## The Application of Dimerization/Cleavage of Anthracenes to Dismantling Adhesion



Yoko Matsuzawa  
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One way to promote recycling is to design products that can be easily disassembled. It is expected that the quality of materials in the recycling loop will be maintained if the product's constituent parts can be disassembled at will, preventing the mixing of different materials. By replacing each part of a product as desired, we can also expect to extend its lifespan.

We have designed and synthesized molecules with anthracene moieties and examined the effects of polymerization/dissociation reactions of anthracenes induced by light or heat on adhesion phenomena in the bulk or at interfaces. The viscous liquid sugar alcohol having multiple anthracene moieties can be polymerized by light at a wavelength that encourages intermolecular dimerization of the anthracenes, leading to solidification. The polymerized solid matter can be returned to its viscous liquid when it is dissociated by UV light exposure (< 300 nm) or heating (< 200 °C). This stimuli-responsive phenomena of the anthracene derivative are promising for use as a removable adhesive. By sandwiching the compound between two pieces of glass and irradiating it with light, polymerization occurs, and adhesion progresses. The adhesive strength can be weakened by dissociation of polymerization through UV light exposure or heating. External stimuli cause liquefaction/solidification phenomena that are heavily influenced by the molecular structure, including the type of sugar alcohol in the basic skeleton and the substitution position of anthracenes. The design of the molecular structure is crucial for functional expression.

Further, we also examined ways to enable the polymerization/dissociation reaction to take place at the interface. A surfactant substituted with an anthracene or its dimer was developed and synthesized. Our study revealed that the adhesion strength can be controlled by altering the anthracene moieties in surface layers with external stimuli. The surfactants with anthracene have the ability to act as a primer for adhesives that are commercially available, which can impart disassembly properties.

In place of mechanical destruction and acid/alkali treatment that might damage the base material, it is preferred to use more mild demolition methods considering future recycling.

Anthracene-containing stimuli-responsive materials are expected to be utilized as adhesives that can be reversible, but physical property optimization is still being investigated.

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# Poster Sessions

P02

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**Georg Winkens**

## Solid solution strengthening in single phase Mo alloys



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In body-centered cubic metals and alloys, screw dislocations are considered to control the strength due to their high critical stress. However, recent experimental and theoretical works on multicomponent solid solutions indicate a similar critical stress for edge dislocations in these alloys. With increasing atomic misfits due to different atomic sizes, the critical stress increases for edge dislocations, until a transition from screw to edge dislocation-controlled strength is achieved. While individual alloys have been identified as either screw or edge dislocation-controlled, the transition has not been observed in a systematic study yet. Consequently, the prerequisites to achieve this transition are not yet known.

While in multicomponent systems superimposed strengthening contributions from precipitation or local atomic ordering might occur, an investigation of binary solid solutions precludes potential problems from chemical complexity. Here, Mo-Ti and Mo-Nb solid solutions were investigated systematically. Both systems cover a similar range of lattice parameters, however, while the lattice parameter in Mo-Ti solid solutions increases strongly non-linearly with Ti content, the one in Mo-Nb changes almost linearly. Accordingly, the former presents a system where both small and large atomic misfits are realized within a single system and the latter serves as reference system with an intermediate misfit value. Mechanical testing from the nanometer to the millimeter scale revealed no significant strength contributions from grain boundaries or oxides potentially formed at grain boundaries. The combination of several chemical analysis methods revealed a significant amount of O dissolved in Ti-rich Mo-Ti solid solutions. As the O impacts the total yield strength, it is corrected for, consistent to the applied strengthening models. The remaining substitutional solid solution strengthening is compared to the models by Maresca and Curtin to identify the strength-controlling dislocation types. While the strength in both systems can be described as controlled by screw dislocation motion, when appropriate energy parameters are used in the models, the parameter-free model for edge dislocation-controlled strength by Maresca and Curtin indicates competitive strengthening in both systems when certain misfit thresholds are surpassed.

These threshold values, when taking the shear modulus into account, allow for a comprehensive screening of binary and multicomponent solid solutions for candidate systems with edge dislocation-controlled strength to aid future model-guided alloy design.

# Poster Sessions

P03

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**Samuel Aeneas Kredel**

## **Preparation of ceramic coatings based on ultrahigh-temperature ceramic nanocomposites from precursors**



Environmental and thermal barrier coatings (EBCs and TBCs) see increasing interest as the requirements of high temperature applications become more and more challenging. In turbines, the current combination of superalloy with zirconia-based TBC is operating at its limits and new material systems need to be designed from ground up in order to achieve a significant rise in operating temperature, that would then lead to increased turbine efficiency. One candidate material class for new protective coatings are polymer derived ceramics. Through chemical modification of commercially available preceramic polymers, single source precursors (SSPs) with enhanced high temperature properties have been prepared and several coatings thereof have been applied on various substrate materials. Thereby, either dense and crack-free thin layers or porous thick layers have been successfully prepared. While showing promising results in first evaluations, their suitability for EBC or TBC application needs further thorough investigation.

*Samuel Aeneas Kredel  
TU Darmstadt, Germany*

# Poster Sessions

P04

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Lukas Korell

## MatCom-ComMat P.7: High-temperature Stability in Harsh Environments



Lukas Korell  
DECHEMA, Germany

To increase the efficiency of turbines they have to run at higher temperatures. That is why new materials has to be developed, which can withstand corrosive atmospheres at high temperatures. Because of their high melting point and good mechanical properties, refractory elements are promising candidates to be used in high temperature applications.

The hot corrosion behavior of the Ni-based alloys which are commonly used in high temperature applications is well studied. It shows two mechanisms which are attributed to the melting of  $\text{Na}_2\text{SO}_4$  (type I) and the formation of eutectics with lower melting points (type II). For the Mo-Based alloys the Mo has an high influence in the corrosion behavior.  $\text{Na}_2\text{MoO}_4$  will form, which has melting point of 687 °C and is able to dilute protective oxides. Also it can form an eutectic with  $\text{MoO}_3$  which melts at around 500 °C. Therefore the system for this alloys is changing from a Na-based to a Mo-based.

In next phase of the research training group MatCom-ComMat, the corrosion resistance of the new developed Mo-based alloys are investigated in a  $\text{SO}_2$ -containing atmosphere at temperatures between 500 °C and 900 °C. After the experiments the sample are analyzed by XRD, SEM and EPMA. The objectives are to observe the development of the corrosion rate and to determine the temperatures regimes (similar to type I and type II for Ni-base) as well as temperature ranges which promote degradation mechanisms of pitting and hot corrosion. In advance test with varying salts (e.g  $\text{NiSO}_4$ ) will be conducted.

# Poster Sessions

P05

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**Federico Ursino**

## Facile synthesis of sulfurized $\text{MoO}_3$ nanostructures from industrial waste powder for energy storage application



*Federico Ursino*  
*University of Catania, Italy*

The climate change requires both new solutions for energy sources and the development of more environmentally friendly and efficient energy storage devices. The treatment of industrial waste to obtain nanostructured materials for energy application can be a promising strategy for mitigating environmental issues. Industrial waste powder rich of Mo attract a lot of interest thanks to the catalytic properties of Mo-based oxides and sulphides. Here, we report a novel, low-cost synthesis consisting in a two-steps hydrothermal process to obtain sulfurized  $\text{MoO}_3$  ( $\text{MoS}_2/\text{MoO}_3$ ) nanostructures starting from Mo-based industrial waste powder. Scanning electron microscopy, Raman spectroscopies and Rutherford backscattering spectrometry have been used for physical-chemical characterization. The first step concerns with the  $\text{MoO}_3$  nanobelts (50-200 nm wide, 10  $\mu\text{m}$  long) synthesis from a peroxy-molybdate solution, obtained by mixing Mo-based starting powder with  $\text{H}_2\text{O}_2$ . The morphology of  $\text{MoO}_3$  nanobelts strongly depends on the hydrothermal bath pH. The  $\text{MoO}_3$  nanostructures have been sulfurized into  $\text{MoS}_2/\text{MoO}_3$  nanocubes (200 nm wide) by a second hydrothermal treatment and with the addition of thiourea in solution.  $\text{MoS}_2/\text{MoO}_3$  nanocubes were sonicated for 12 hours and tested for energy storage applications using Cyclic Voltammograms (CV) and Galvanostatic Charge-Discharge (GCD) measurements within neutral electrolyte (1 M  $\text{Na}_2\text{SO}_4$ ). High specific capacitance values were recorded for these nanostructures, 173  $\text{F g}^{-1}$  and 215  $\text{F g}^{-1}$  respectively at 5  $\text{mV s}^{-1}$  and 0.5  $\text{A g}^{-1}$ . These results open a way to large scale application of recycled materials for energy storage.

# Poster Sessions

P07

**Gabriely Falcão**

## Development of ductile and oxidation resistant Cr-Mo-Si solid solution alloys



*Gabriely Falcão  
Karlsruhe Institute of Technology (KIT), Institute for Applied Materials IAM*

To further improve the efficiency of turbines, it is inevitable to develop new high temperature structural materials, which can exceed the operating temperatures of currently used Ni-based super alloys. For these applications, Mo-based alloys are particularly promising as they exhibit superior strength and creep resistance. Extensive efforts in terms of alloy design, microstructure control, and component analysis were performed to develop for example advanced Mo-silicide alloys.

While strength and creep resistance in Mo-silicide alloys are already superior to Ni-based superalloys, oxidation/corrosion resistance, required to withstand the combustion atmosphere, and ductility/toughness, needed for failure tolerance, still display substantial barriers for the application of these candidate materials. Mo and most of its alloys suffer from catastrophic oxidation ("pecking") above 500°C by the oxidation along grain boundaries to MoO<sub>3</sub>, which evaporates due to its high vapor pressure. The progress of oxidation leads to a quick disintegration of parts. In contrast, Cr is usually considered as passivating element that forms dense Cr<sub>2</sub>O<sub>3</sub> scales. However, Cr and Cr-based alloys suffer from scale spallation and nitridation when being exposed to air at high temperatures. Any successful attempt to address oxidation resistance in these alloy systems came along with obvious deterioration in ductility as usually brittle intermetallic phases are needed to provide reservoirs for passivating elements.

Recently, an outstanding combination of resistance against oxidation in air in the critical temperature range and ductility even at room temperature was identified for an arc melted Cr-Mo-Si solid solution. In the present contribution, the design strategy was extended to varying Mo contents and microstructural conditions, see Figure 1 for an illustration of the compositions investigated. These alloys were produced using arc melting process exhibiting a dendritic microstructure in the as-cast condition. In order to homogenize the microstructure, high temperature, long-term annealing treatments were performed. The investigations focused on the critical properties: (i) resistance against pecking, nitridation and scale spallation at elevated temperatures of 800 °C and 1100 °C as well as (ii) ductility at low temperatures.

# Poster Sessions

P08

Dharma Teja Teppala

## Mechanochemical synthesis and characterization of compositionally complex transitional metal oxides



Dharma Teja Teppala

Compositional complexity in ceramics represents an emerging area of materials consisting of medium entropy, high entropy and non-equimolar compositional ceramics. Compositionally complex oxides consist of at least three or more cationic species randomly distributed on the cationic sublattice, resulting in the formation single-phase compounds with rather unique properties.

Several methods such as solid-state synthesis, polymeric stearic entrapment, co-precipitation, nebulized spray pyrolysis, PVD, sputtering were used to synthesize compositionally complex ceramics, with an disadvantage of either requiring high temperatures for obtaining single phase leading to grain growth or requiring an specialized setup for the synthesis.

In this present work, a simple solvent deficient synthesis method was applied to synthesize two classes of oxides i.e., spinel-type  $(\text{Co}_{0.33}\text{Fe}_{0.33}\text{Mn}_{0.33})\text{O}_4$ ,  $(\text{Co}_{0.25}\text{Fe}_{0.25}\text{Mn}_{0.25}\text{Ni}_{0.25})\text{O}_4$ , and  $(\text{Co}_{0.2}\text{Cr}_{0.2}\text{Fe}_{0.2}\text{Mn}_{0.2}\text{Ni}_{0.2})\text{O}_4$  oxides as well as bixbyite-type  $(\text{La}_{0.16}\text{Ce}_{0.16}\text{Pr}_{0.16}\text{Nd}_{0.16}\text{Sm}_{0.16}\text{Gd}_{0.16})\text{O}_3$  by mechanochemically reacting the a mixture of the respective hydrated metal nitrate salts with ammonium bicarbonate. The resulting mixture of hydroxides and (hydroxy)carbonates was rinsed with water in order to remove ammonium nitrate and subsequently calcined at a series of temperatures ranging from 500 °C to 1000 °C resulting in single-phase spinel- and bixbyite-type oxides.

Structural characterization of the ceramics by vibrational spectroscopy and X-ray diffraction proved the formation of single-phase oxides at the considered temperatures. Moreover, temperature-dependent in-situ XRD was used to rationalize the conversion of the precursors into the respective oxides.

The solvent deficient synthesis method can be easily upscaled without any usage of solvent in synthesis of the oxide ceramics, thus being a highly attractive preparative approach as compared to other synthesis methods for oxides.



# Poster Sessions

P09

Minoo Boroojerdi

## Single source precursor synthesis of ceramic composites for UHTC application



Minoo Boroojerdi  
TU Darmstadt

Ultra-high temperature ceramics consists of borides, carbides, and nitrides of group 4 and 5 transition metal elements. These compounds are characterized by their covalent solid bonds, which lead to high hardness, stiffness, and a melting point of over 3000°C. This material class holds significant interest for engineering applications, particularly in space and hypersonic re-entry components. However, their challenging processing hinders widespread use in conventional engineering sectors. Another limitation is their moderate oxidation resistance; for instance, HfC initiates oxidation around 550°C, forming a porous oxide scale. Strategies to mitigate these limitations include incorporating silica-forming additives to generate a stable SiO<sub>2</sub> scale and forming a glassy borosilicate layer. Alternatively, the polymer-derived ceramics (PDCs) route offers a promising avenue for processing UHTCs at lower temperatures and pressures, with composites containing high silica former content being accessible. In this work, the commercially available precursors Durazane 1800 (SiCN precursor) and SMP 10 (SiC precursor) were modified with transition metals of hafnium and tantalum in a ratio of approximately 7:3 to obtain liquid precursors. The preceramic precursors displayed excellent processability in coating experiments, yielding crack-free and homogenous layers. The coatings exhibited exceptional resistance to extreme temperature fluctuations without any spallation during repeated rapid thermal cycling. Amorphous bulk samples synthesized analogously displayed excellent short-term oxidation resistance and low thermal conductivity (below that of 8YSZ), positioning Six (Hf<sub>0.7</sub>Ta<sub>0.3</sub>)w(Bvar)CyNz, a promising candidate for high-temperature application. Furthermore, highly dense samples of SiC/(Hf<sub>0.75</sub>Ta<sub>0.25</sub>)C(N)/(B)C were produced via Spark Plasma Sintering (SPS) consolidation for in-depth analysis of intrinsic thermal and mechanical properties. Outstanding nanocomposites were produced and characterized by a finely homogeneous distribution of UHTC phases in SiC-Matrix. The samples exhibited extreme macro hardness (31GPa) exceeding that of commercial superhard materials and very low thermal conductivity for SiC-based materials.

# Poster Sessions

P10

**Sri Rathinamani Ramdoss**

## Influence of interfaces on the plastic deformation of Mo-Si-Ti alloys



*Sri Rathinamani Ramdoss*  
KIT

Mo-Si-Ti alloys, particularly the eutectic composition Mo-20Si-52.8Ti (at%), have been extensively studied due to their exceptional resistance to oxidation and creep [1,2]. The composition yields a body-centered cubic (BCC) disordered Mo-rich solid solution and an intermetallic hexagonal  $(\text{Ti},\text{Mo})_5\text{Si}_3$  phase. Three distinct microstructures were obtained from different processing routes: arc melting (AC), arc melting followed by heat treatment at 1600°C for 150 hours (HT) and direct energy deposition (DED). The microstructures from different processing routes have been displayed in Fig. 1a-e. In high-temperature compression tests with various interphase boundary spacings, finer microstructures exhibited lower yield strength, contrary to expectations (Fig. 1f).

One possible explanation is the presence of precipitates at phase boundaries affecting strain transfer to investigate the impact of the interfaces in the plastic deformation and their contribution to the strength of the two-phase alloy the nanoindentation testing has been conducted over the three sample sets and effect of solid solution strengthening proffered by each phase present in the microstructure is elucidated.

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# Poster Sessions

P11

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**Katharina Beck**

## Microstructure and hot corrosion behavior of Cr-Mo-Si alloys



Currently used Ni-base alloys reach the limit of their operation temperature beyond 1150°C, therefore new material systems are needed. Promising alternatives are Mo-based alloys, which exhibit very high melting points combined with a high mechanical strength. However, these alloys are prone to pesting, which describes the total disintegration of metal bulk material into powder and volatile corrosion products, at temperatures below 1000°C. In a similar temperature range between 650°C and 950°C Na and SO<sub>2</sub>-containing flue gases lead to fast material degradation by hot corrosion. The type II hot corrosion behavior (2.5 mg/cm<sup>2</sup> Na<sub>2</sub>SO<sub>4</sub> deposits, synthetic air/0.1 % SO<sub>2</sub> atmosphere at 700°C up to 100 h) of two uncoated and Cr-coated Mo-Si-Ti alloys (eutectic Mo-20.0Si-52.8Ti and eutectoid Mo-21.0-34.0Ti) was investigated. Both alloys were subject to type II hot corrosion attack. The higher Ti content of the eutectic Mo-20.0Si-52.8Ti significantly reduced the formation of Mo oxides led to an improved hot corrosion behavior compared to the eutectoid Mo-21.0-34.0Ti.

*Katharina Beck*  
*DECHEMA; Germany*

# Poster Sessions

P13

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**Dr. Romy Auerbach**

## **DigInform – a Digital Information Management System towards a Circular Economy in the Chemical Industry**



The project DigInform developed an information management system (IMS) for various stakeholders in the chemical industry and the waste disposal sector. The aim was to identify new recycling strategies, promote the networking of stakeholders along the value chain and demonstrate the added value of information exchange for the implementation of recycling strategies. The platform also serves as a marketplace for by-products or faulty batches. The exchange between producers and disposers of by-products was standardized and accelerated by the IMS. The transferability to other material flows and use cases was examined and the effects on climate protection and resource efficiency were quantified.

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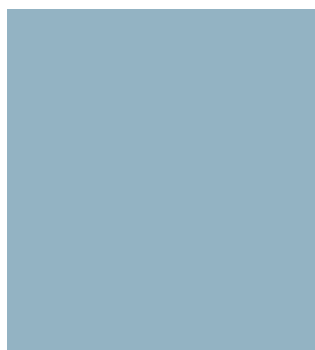
# Poster Sessions

P14

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Moritz Thiem

## The instabilities of thermoelectric high ZT SnSe compounds



*Moritz Thiem*  
*TU Darmstadt, Germany*

The SnSe compounds have emerged as promising candidates for thermoelectric (TE) applications, primarily due to their remarkable achievement of a high ZT value and the relative abundance of their constituent elements. However, a significant disparity in the performance of polycrystalline SnSe compounds has been observed, and the underlying mechanisms remain unclear. This study focuses on the impact of sintering temperature on the thermoelectric properties of both Br-doped and undoped SnSe materials. We achieved a ZT value of 1.04 at 873 K through a systematic investigation. However, our findings reveal a critical challenge in the long-term stability of SnSe-based thermoelectric materials. The peak ZT values observed in the initial measurements are not sustainable, as the thermoelectric performance experiences a decline during multiple heating-cooling cycles. This issue is further underscored by extended annealing experiments, which resulted in a substantial ZT decrease of approximately 50%. These outcomes emphasize the need for a comprehensive understanding of the long-term stability of SnSe materials in thermoelectric applications. Additionally, they highlight the importance of conducting heating-cooling measurements in TE systems, particularly when striving to achieve and maintain high ZT values.

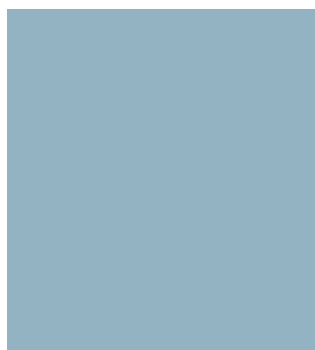
# Poster Sessions

P15

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**Jinxue Ding**

## Applying entropy engineering strategy in $\text{TiS}_2$ -based thermoelectric materials



Jinxue Ding  
TU Darmstadt

Taking inspiration from high-entropy alloys, our research group is recently interested in applying an entropy engineering strategy to design high-performance and sustainable thermoelectric materials. The entropy-stabilized single-phase structures can preserve the long-range order of atomic arrangement with weak phase-boundary electron scattering, thereby maintaining the electrical transport framework. At the same time, short-range disorder in high-entropy materials arises due to severe lattice distortion caused by the mismatch of ionic mass, size, and bond state. Titanium disulfides ( $\text{TiS}_2$ ) has emerged as a highly promising material in thermoelectrics owing to its economic viability and sustainable characteristics. Herein, we first developed entropy-engineered  $\text{TiS}_2$  by equal mole doping at Ti sites with Zr, Nb, and Ta. The entropy engineering can largely reduce its lattice thermal conductivity, but a significant decrease in Seebeck coefficient is also observed, because of the higher carrier concentration resulting from high oxidation states (+5) of Ta and Nb. These results inspired us to perform equivalent doping with Se at S sites and incorporate small amounts of Zr, Nb, and Ta at Ti sites. The as-synthesized compositional complex  $\text{TiS}_2$ -based materials can retain their large power factor while exhibiting reduced lattice thermal conductivity.

# Poster Sessions

P16

Md Mahmudul Hasan

## Sustainable Management of Nd-Fe-B Magnet Waste Streams: Enhancing Supply Security and Circular Economy in High-Tech Applications through Effective Functional



Md Mahmudul Hasan  
Fraunhofer IWKS; Germany

The exceptional properties of Nd-Fe-B magnets have positioned them as vital components in numerous essential technologies, playing key roles in energy applications, wind turbine generators, motors for hybrid and electric vehicles, and consumer electronics [1]. However, challenges arise due to the reliance on rare earths (RE) in their production, posing concerns related to RE supply security and market dynamics. Furthermore, the environmental issues associated with RE mining exacerbate these challenges. Extensive research has been conducted to minimize the utilization of heavy rare earths (HREs) in magnets [2] and implement effective recycling methods for existing REEs sourced from industrial residues, pre-consumer scrap, and end-of-life products [3,4].

our study emphasizes the effective and functional recycling of high-performance Nd-Fe-B magnets obtained from diverse waste streams of scrap magnets. At the same time, it seeks to showcase to potential industries that primary magnets can be substituted in various applications with more sustainable recycled magnets, all without compromising performance. This shift not only decreases costs and supply-related risks but also plays a role in fostering a more sustainable circular economy.

To attain effective functional recycling, we gathered Nd-Fe-B magnets from diverse end-of-life products like electro-motors, wind turbines, and magnetic resonance imaging (MRI) magnets, along with production wastes. These components were thoroughly analyzed and then subjected to the recycling process following the short loop recycling route (Functional Recycling).

The recycled magnets' properties were assessed in comparison with the target values of the primary magnets extracted from the devices under investigation (industrial motors, E-Scooters, lawn mower robots, cleaning robots, e-bikes, e-scooters, and hoverboards). The results showed that recycled magnets possess magnetic properties that are adequate, rendering them suitable substitutes for primary magnets in various applications. Further testing on test benches confirmed that incorporating recycled magnets, such as in e-bikes, e-scooters, and hoverboards, does not compromise performance and is indeed entirely feasible.

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# Poster Sessions

P17

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**Dr. Wenjie Xie**

## **Pursuing Sustainable Thermoelectrics**



*Dr. Wenjie Xie  
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Thermoelectricity offers a direct and highly efficient approach for converting heat into electricity, relying on two key factors: Carnot efficiency and the materials-dependent property, ZT. In the last two decades, tremendous efforts have been made to develop high ZT thermoelectric materials, and the bulk ZT has reached above 3. Energy converters for renewable or sustainable energy technologies have to be based on materials that are not a burden to the environment, do not contain critical elements and guarantee a short energy payback time. Besides improving the conversion efficiency and other performance factors, sustainability has to be considered when designing novel thermoelectric materials and devices. In this work, we will introduce novel synthesis strategies for oxide and silicon-based thermoelectric materials. We will delve into the concept of Entropy Engineering, a method that can extend the lifetime of (oxide) thermoelectric materials. Moreover, we will showcase one example where waste Si from the solar cell industry is transformed into valuable products, specifically in the synthesis of  $\text{MnSi}_{1.75}$  alloy. This underscores the potential to convert waste into valuable resources, contributing to both sustainable energy and responsible material usage.



# Poster Sessions

P18

Vidushi Galwadu Arachchige

## Alternative manufacturing of ZrNiSn half-Heusler thermoelectric



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Traditionally, thermoelectric materials are manufactured as blocks of material using spark plasma sintering or hot pressing. These blocks have to be further processed to form the legs for device assembly. Thus, the production of thermoelectric devices is a long, laborious and resource demanding chain of process steps. [1] However, alternative methods of manufacturing were developed over the last decades that promise to reduce the production steps and conserve resources by reduction of energy consumption and efficient use of the material. We present our preliminary work on manufacturing the well-established half-Heusler thermoelectric material ZrNiSn using two such techniques: Additive manufacturing via selective laser melting as a near-net shape manufacturing technique [2] and electro sinter forging as a resource-efficient [3] alternative to spark plasma sintering and hot pressing.

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# Poster Sessions

P19

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**Xia Wang**

## Spin-controlled electron transfer in topological chiral semimetals for high-performance oxygen catalysis



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Spin-controlled electron transfer in topological chiral semimetals for high-performance oxygen catalysis  
Xia Wang, Binghai Yan and Claudia Felser

The oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are four-electron transfer processes that involve product in singlet ground states ( $1\Delta$ ) as well as oxygen molecules in triplet states ( $3-g$ ). This spin-dependent multi-electron transfer process results in sluggish reaction kinetics, which severely limits the efficiency of sustainable energy conversion systems such as fuel cell, water splitting and metal-air batteries. To address this issue, it is essential to control and understand the spin-dependent electron transfer process at the atomic active sites for oxygen catalysis, but this has not been addressed due to the lack of intrinsically chiral catalysts. Herein, we synthesized topological chiral semimetals as ORR/OER electrocatalysts and quantified the spin contributions to the activity.

Our work reveals the pivotal roles of chirality and SOC in spin-dependent catalytic processes, facilitating the design of ultraefficient chiral electrocatalysts.

# Poster Sessions

P20

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**Federico Ursino**

## Low-cost synthesis of nanostructured catalysts for Oxygen Evolution Reaction and Hydrogen Evolution Reaction from Molybdenum industrial waste powder



*Federico Ursino*  
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The increasing worldwide energy request is a new scientific challenge, because our goal is satisfying the energy demand preserving our planet, through more sustainable technologies. New studies are done in according to the Critical Raw Materials (CRMs) list published by European Union, this is a good practise as well as the reuse of industrial waste. Among transition metals, molybdenum (Mo) attracts a large interest thanks to its characteristics and the possibility to use like catalytic material. This work concerns with a novel process to obtain Mo-based nanostructures catalysts for water splitting application by industrial waste powder, e.g. for Oxygen Evolution Reaction (OER) and Hydrogen Evolution Reaction (HER). MoO<sub>3</sub> nanobelts (50 nm thick, 200 nm width, about 10 μm long) were synthesized by hydrothermal (at 180 °C for 3 h) on a peroxide solution of Mo industrial waste powder. MoO<sub>3</sub> nanostructures were employed as anode for OER, it was studied the effect of growth parameters on the electrochemical performances, it was recorded also a promising overpotential of 324 mV at 10 mA cm<sup>-2</sup> and a Tafel Slope of 45 mV dec<sup>-1</sup> around 10 mA cm<sup>-2</sup> in alkaline conditions. Sulfurized MoO<sub>3</sub> nanostructures were synthesized through a second hydrothermal step, and they were employed as cathode for HER. Again, the growth parameters were optimized to improve the electrocatalytic activity of the nanostructures. An overpotential of 213 mV at 10 mA cm<sup>-2</sup> and a Tafel Slope equal to 68 mV dec<sup>-1</sup> around mA cm<sup>-2</sup> in acidic electrolyte. This work opens a route for the application of Mo-based industrial waste for green hydrogen production.

# Poster Sessions

P21

Jueun Jang

## Recycling of valuable cathode materials from spent Li-ion batteries based on deep eutectic solvent leaching with oxalate chemistry



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The advent of lithium-ion batteries (LIBs) has revolutionized portable electronics, electric vehicles (EVs), and energy storage systems (ESS) due to their impressive energy capacity, minimal self-discharge, and absence of memory effect. With the rising demand for LIBs, an overflow of waste batteries is anticipated shortly. Utilizing deep eutectic solvents (DES) as a potential greener alternative to conventional methods employing inorganic acid is under investigation in the hydrometallurgical process to recycle LIBs. DESs facilitate metal dissolution by forming stable complexes supported by hydrogen bonds between the hydrogen bond acceptor (HBA) and hydrogen bond donor (HBD), offering feasible avenues for effective metal extraction from LIBs while possibly minimizing environmental impact.

In this contribution, choline chloride (ChCl) and oxalic acid (OxA), acting as the HBA and HBD, respectively, were combined in a 1:1 molar ratio to form a DES. Oxalic acid has emerged as a promising reagent for the recovery of metal mixtures from spent LIBs under mild reaction conditions, demonstrating superior leaching efficacy and selectivity. The proposed recycling process with oxalic acid-based DES offers a reductant and precipitant-free approach for recovering valuable metals from spent LIBs. Additionally, leveraging oxalic acid-based DES can streamline processes and reduce secondary pollutants, as oxalate can serve as a leaching agent, reductant, and precipitant.

Different cathode materials with various chemical compositions were utilized for cathode regeneration. Metal oxalates were produced with extraction efficiencies of 99% for Ni, 97% for Co, and 77% for Mn in the case of  $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$  cathode (NMC811). Metal oxalate precursors were regenerated with additional Li source and following high-temperature calcination, resulting in well-crystallized cathode active materials. In electrochemical testing, the regenerated LCO, NMC811, NMC433 Scrap, NMC622 BM, and NMC811 BM exhibited the capacity retention were to 84, 52, 98, 64 and 4 %, respectively, with coulombic efficiencies around 98 %, after 50 cycles at 0.5 C.

Li persisted in the supernatant due to its high solubility under oxalic acid-based DES unlike Ni, Co, and Mn. Attempting Li extraction using a basic precipitant  $\text{Na}_2\text{CO}_3$  resulted in sodium oxalate rather than lithium carbonate. A comparative leaching experiment was also conducted, comparing oxalic acid-based DES with oxalic acid alone. Complete leaching proceeded more rapidly with oxalic acid-based DES, attributed to the hydrogen bonding within the DES, coupled with the concurrent presence of chlorine and oxalate anions, which collectively enhance the leaching kinetics. Furthermore, the DES demonstrated reusability for three cycles without requiring ChCl or OxA addition, while maintaining high metal leaching efficiency.

The findings indicate that the utilization of ChCl:OxA DES for hydrometallurgical cathode material regeneration facilitated rapid and efficient leaching of transition metals such as Ni, Mn, and Co. leading to the regeneration of cathode active materials with satisfactory electrochemical characteristics. Furthermore, the feasibility of recycling DES has also been demonstrated. The potential of this regeneration process as a promising industrial alternative can be considered if quality control of blackmass in the pretreatment stage, the reduction of residual lithium compounds and the increase in lithium recovery can be achieved.

# Poster Sessions

P22

**Tommi Aalto**

## Towards Carbon Free Fluoride Ion Batteries



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Fluoride-Ion-Batteries (FIBs) promise high specific capacities and energy densities, some even higher than current lithium-ion batteries [1]. However, good cyclic stability using intercalation-type cathode materials could only be achieved by drastically limiting the operational capacity of FIBs, due to parasitic side reactions including the carbon additive [2]. While carbon is an essential additive to the electrode composites to ensure proper electronic conduction networks, it can easily be oxidized leading to loss of conductivity, thereby degrading the conductive matrix of the composite. In order to achieve high cyclic stability as well as high specific capacities, the carbon-side reactions in FIBs need to be either suppressed or avoided altogether.

A promising candidate for replacing carbon in the role of the conductive additive in solid-state electrode composites are conductive oxides. If no further oxidation of metal cations is possible, the only oxidative side reaction possible is oxygen evolution, which would only happen at voltages far above the working potentials of FIB cathodes and would also be associated with high overpotentials due to kinetic limitations of the oxygen evolution reaction. Therefore, the use of conductive oxides as a substitute for carbon could enable an oxidatively stable conduction matrix for fluoride ion battery cathodes.

This work presents the path towards carbon-free cathode composites for fluoride ion batteries using conductive oxide nanoparticles as a substitute for carbon additives. Nanoparticles have a low percolation threshold due to their small size [3], which enables them to occupy the free volume between active material and solid electrolyte particles. Therefore, good percolation and contact of all particles in the composite can be achieved with a comparably low volume fraction of nanoparticles. The use of antimony-doped tin oxide nanoparticles provided a side-reaction free cathode composite for fluoride ion batteries, enabling the reversible electrochemical fluorination of the active material within a stable matrix.

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# Poster Sessions

P23

Hyunjung Lim

## Microwave-assisted Regeneration of Li-ion Battery Cathode Active Material by Deep Eutectic Solvents



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The lithium-ion battery (LIB) industry has emerged as a cornerstone of modern technological advancement, powering the widespread application of portable electronic devices, electric vehicles (EVs), and renewable energy storage systems. As the demand for LIBs keeps growing, concerns about resource depletion, environmental impact, and waste management have become increasingly prominent in discussions. One crucial aspect of the LIB lifecycle that demands attention is the recycling of cathode active materials. From conventional processes such as hydrometallurgical and pyrometallurgical methods to innovative techniques like direct recycling of cathode materials, the exploration of recycling methods offers insights into advancing the circular economy for LIBs and reducing dependency on raw materials. The main objective of this study is to improve the recycling process of cathode active materials extracted from LIBs by hydrometallurgical manner, substituting conventional solvents with potentially green alternatives known as deep eutectic solvents (DESs).

The dissolution and leaching of metal components from the cathode active materials are crucial steps in the hydrometallurgical recycling process, and the unique ability of DES to solvate a wide range of metal species, combined with its tunable physicochemical properties, makes it a promising solvent for recycling cathode active materials. In this work, DESs composed of choline chloride (ChCl) as hydrogen bond acceptor (HBA) and three distinct types of hydrogen bond donors (HBDs), ethylene glycol, urea, and oxalic acid, were incorporated. The dissolution steps for cathode active materials in DESs were systematically executed, employing microwave-assisted heating methods to enhance the dissolution reactions and its efficiencies. This study revealed that  $\text{LiCoO}_2$  (LCO) and  $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$  (NMC 811) dissolved effectively in ChCl:oxalic acid DES, achieving extraction efficiencies of more than 99.6 % for cobalt and nickel, and 96.7 % for manganese. The microwave-assisted solvothermal process required shorter reaction time compared to conventional heating methods, with the process completing in 30 min at 120 °C. The extracted metal oxalate precursors further reacted with different amounts of lithium source to regenerate LCO. The initial specific discharge capacities of the regenerated LCO closely matched those of pristine LCO, ranging from 129.6 to 132.1 mAh  $\text{g}^{-1}$  at 0.1 C, with coulombic efficiencies between 95 % and 98 %, and achieving capacity retention of 74.0 % after 100 cycles at 0.5 C.

Despite being considered environmentally friendly and exhibiting good performance, these processes accompany their own challenges to be overcome. This study also highlights the challenges associated with the industrial application of DES, including its high viscosity, and limited thermal and chemical stability. Moreover, parameter studies on lithium loss in the modified process utilizing microwave-assisted heating methods have been conducted, requiring future advancements in LIB recycling processes. These findings emphasize the significance of acknowledging and mitigating potential risks inherent in recycling processes while also considering sustainability in the development of Li-ion battery recycling technologies.

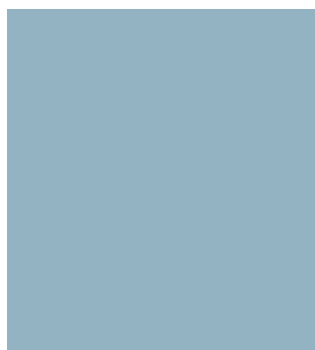
# Poster Sessions

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**Kerstin Wissel**

## Recycling of solid-state batteries



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*Germany*

All-solid-state batteries (ASSBs) are currently developed at high pace and show a strong potential for market introduction within the next years. Several solid electrolyte classes (e.g. oxides, sulfides and halides) used in these batteries are intensively studied with a focus on further optimization of the synthesis and the electrochemical performance.

With the growing significance of ASSBs, investigations of their sustainability and the development of suitable recycling strategies for spent cells allowing for an efficient recovery of critical elements (lithium, cobalt and other transition metals, etc.) become a matter of increasing importance. However, so far only a limited number of studies have been conducted on the recycling of ASSBs. For conventional lithium-ion batteries, there is a broad variety of established approaches including pyrometallurgical, hydrometallurgical, and direct recycling methods. While these methods can be partly adapted to derive recycling strategies for ASSBs, it is crucial to recognize that these approaches cannot be directly applied to ASSBs due to their unique properties, which can be in many cases primarily attributed to the chemical nature of the solid electrolyte employed in these batteries (i.e., moisture and air stability of the electrolyte). Additionally, for conventional lithium-ion batteries, recycling methods are often limited to the recovery of the most-valuable critical elements from or the regeneration of the active cathode materials. In contrast, for ASSBs, there is a need to process complex mixtures comprising of active electrode materials, solid electrolytes, binders, etc. containing a multitude of valuable elements that have to feed back into economic cycle. This leads to an increased complexity of the recycling processes. In this contribution, possible concepts and challenges for the recycling of ASSBs with different electrolyte classes are discussed based on various model mixtures. It is shown that, with respect to the economic value, not only resource and/or element-specific aspects but also the chemical value of individual battery components related to required energy-intensive synthesis procedures should be considered. Depending on the detailed composition of an ASSBs, different approaches are described relying either on the extraction and recovery of valuable elements (requiring energy-intensive re-synthesis of individual battery components later on) or on the separation and/or regeneration of battery components while maintaining and/or reforming the original state of the components (without disassembling them into individual constituents down to atomic levels).

# Poster Sessions

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Dennis Michael Jöckel

## Feasibility study and life cycle assessment of boron-assisted direct cathode recycling of $\text{LiCoO}_2$ for Li-ion batteries



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With global surface temperatures already surpassing pre-industrial levels by 1.5 °C in the last 12 months [1] and greenhouse gas emissions reaching a record high in 2023 [2], it has never been more urgent to rapidly decarbonise human activities. One of the most promising technologies to reverse these trends is the electrification of industries. For this purpose, especially in the traffic and transport sector, Li-ion batteries (LIBs) will play an important role. However, due to the complex chemistry and variety in cathode materials, LIBs are difficult to recycle. In 2022 only approximately 5% of all LIBs were recycled [3]. Besides the traditional and highly resource intensive approaches (hydrometallurgy and pyrometallurgy), direct recycling of cathode active materials continues to receive attention for being supposedly more sustainable and resource efficient [4]. Unfortunately, direct recycling has not yet proven to be commercially viable. Here, boron (B) substitution which is a method known to improve stability of pristine LIB cathodes [5–7] is proposed as modification strategy to facilitate and scale up direct recycling. Whether the technology is easily scalable and environmentally beneficial, when compared to the synthesis of fresh LIB cathode material, has yet to be determined. Our study aims to shed light on the feasibility of boron-assisted direct recycling of cathode active materials from spent  $\text{LiCoO}_2$ -based LIBs. The investigated approach involves planetary ball milling, B-substitution, and subsequent thermal treatment (700°C) of spent pre-treated Co-rich black mass. In order to investigate structural changes and property differences in the treated materials, the characterisation methods X-ray diffractometry (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray (EDX) spectroscopy, and thermogravimetric differential scanning calorimetry (TG-DSC) will be utilised. Furthermore, to quantify the environmental impact caused by employing this technology, a life cycle assessment (LCA) will be conducted. The goal of this approach is to provide further decision support on which methodology to choose for direct recycling. To compare different modelled systems with the synthesis of fresh  $\text{LiCoO}_2$  (LCO), the function of each process will be the production of LCO, while the system boundaries will be “cradle-to-gate”, starting after the end-of-life stage of used cathode active materials. In this LCA approach, it is assumed that each LCO output will have the same quality. As functional unit the production of 1 g of LCO is selected, respectively. For the inventory analysis the direct recycling approach will be modelled in detail based on data directly collected from experiments conducted on laboratory scale. To assess its broad environmental footprint in a midpoint-analysis, impact categories recommended by the International Life Cycle Data system (ILCD) will be applied. Finally, limitations and sensitivities of the model will be addressed to critically reflect on the results of this study.

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# Poster Sessions

P27

**Samuel Meles Neguse**

## The Effects of Boron on Li-ion Batteries Recycling Processes



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Lithium-ion batteries (LIBs) play a pivotal role in the modern energy revolution. Consequently, it is expected that the amount of end-of-life (EOL) batteries will increase significantly due to the increasing demand for LIBs in the near future. For example, it is estimated that by 2030, there will be approximately 140 million electric vehicles on the road, therefore, making environmentally sustainable friendly recycling methods for spent LIBs a necessity.[1] Current commercially applied recycling methods are pyro- and hydro-metallurgy. While pyrometallurgy focuses on high-temperature processes, such as smelting to extract metals, hydrometallurgy utilizes acids and extractants to leach and precipitate metals into precursors for regenerated cathode active materials. One of the most environmentally friendly recycling approaches is the direct recycling of spent cathode materials. Direct recycling is an approach, in which spent cathodes are not recycled by destroying the structure, but rather by repairing it and removing the impurities and defects in the cathode active material, which causes major capacity loss.[2] It is an alternative to conventional recycling processes, since it does not need high energy inputs or the usage of toxic solvents. However, the industrial implementation of direct LIB recycling still requires large research efforts to understand the correlations between defect formation during operation and the possible material regeneration. In this context, boron substitution has demonstrated better performance of pristine cathode materials, due to enhanced Li diffusion, increased stability during extended (dis)charge cycles, and inhibition of cation anti-site defect formation. [3] By leveraging this set of insights, this study investigates the incorporation of boron as substituent into the direct recycling process of spent cathode active materials. The focus will be on the doping effects of cathode active materials by various boron compounds. Eventually, demonstrating applicability to black mass originated from various spent LIBs as important intermediate product during battery recycling. The proposed direct recycling process for spent cathode active materials involves the re-lithiation of the materials in combination with the introduction of beneficial morphological effects using different boron sources. By systematically varying the boron sources and their concentration together with well-adjusted experimental parameters such as milling and heat treatment conditions, the impacts on the performance of regenerated cathode active materials will be presented.

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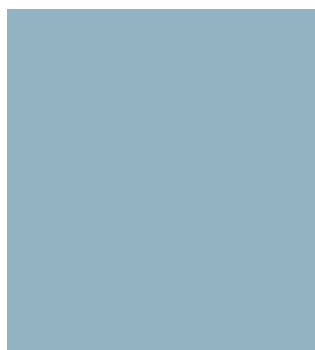
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# Poster Sessions

P28

## Rashid Aasir

### Recycling of Hydrogen Tolerant Oxygen Transport Membranes with Integrated Life Cycle Assessment for Plasma-assisted CO<sub>2</sub>-Conversion



Rashid Aasir  
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With the increase in scarcity of resources, there is a need to integrate sustainability metrics into materials development. The often-followed approach of performance specific materials development does not consider the possible threats to human health and environment posed by the materials use and process emissions. The incorporation of material circularity and materials substitution alongside life cycle assessment (LCA) into materials development is necessary especially for systems which involve usage of critical raw materials such as cobalt (Co), rare earth elements like lanthanum (La), etc. An emphasis on developing (chemical) recycling techniques and material substitution is essential to enhance the life expectancy of such materials. LCA can act as an imperative tool in tracking the associated emissions involved in the materials development and assessing the possible impact on human health and environment.

In the context of oxygen transport membranes (OTM) for CO<sub>2</sub> conversion, using the combined approach of performance and sustainability in the material design phase is sensible, given the regular use of Co and La to impart an increased tolerance against CO<sub>2</sub> without affecting the oxygen permeation. Plasma-assisted CO<sub>2</sub> conversion technology is an emerging technology which can be used for chemical transformation of CO<sub>2</sub> into value added chemicals such as methanol, etc [1]. This technique lays focus on sustainability and with the help of OTMs converts CO<sub>2</sub> into CO and O<sub>2</sub>. The OTMs strongly minimise recombination to CO<sub>2</sub> by maintaining the oxygen partial pressure in the required range within the plasma system. The CO produced can be further utilised by reacting with green H<sub>2</sub> to produce methanol. The OTMs in the plasma system would continuously be interacting with CO<sub>2</sub> and H<sub>2</sub> and thus require to be tolerant against H<sub>2</sub> as well in addition to CO<sub>2</sub>. The (La,Ca)(Fe,Co)O<sub>3-d</sub> system, in particular, in one of its variants La<sub>0.6</sub>Ca<sub>0.4</sub>Co<sub>0.2</sub>Fe<sub>0.8</sub>O<sub>3-d</sub> (LCCF\_6428) with reduced Co content, has shown good tolerance to CO<sub>2</sub> and H without oxygen permeation losses [2,3]. With the presence of Co and La, a chemical recycling pathway was developed using microwave assisted dissolution of the CO<sub>2</sub>/H<sub>2</sub> plasma exposed membrane followed by ultrasonic spray synthesis (USS). This technique uses deionised water as solvent and avoids complexing agents such as citric acid, ethylaminetetraacetic acid, etc, which generate greater process emissions comparatively.

The oxygen permeability of the recycled membrane was 83% of the primary membrane and remained tolerant to H<sub>2</sub> upto 600 °C as well. LCA of the recycling process was compared with primary synthesis to assess its environmental feasibility. The results revealed a higher environmental impact (EI) for recycling process when compared to primary synthesis largely due to higher energy consumption despite lesser degree of scarce resource utilisation which reflects on the need to transition towards cleaner and greener sources of energy.

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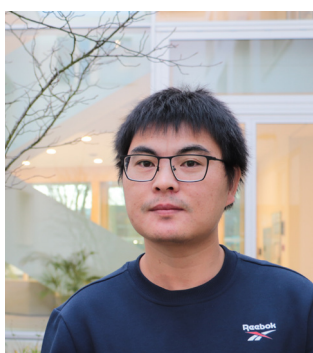
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# Poster Sessions

P29

Dr. Guoxing Chen

## A novel plasma-assisted hollow fiber membrane concept for efficiently separating oxygen from CO in a CO<sub>2</sub> plasma



Dr. Guoxing Chen  
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Plasma-based technologies providing extremely flexible ‘turnkey’ applications are increasingly attracting interest in renewable energy usage and CO<sub>2</sub> conversion into carbon neutral fuels [1-2]. Here, we report a breakthrough concept combining plasma and mixed ionic-electronic conductor, hollow fiber membranes for significantly enhancing the oxygen permeability which may stimulate the CO<sub>2</sub> conversion by direct product separation. Several CO<sub>2</sub>-tolerant oxygen transport membrane (OTM) materials with high oxygen permeation fluxes have been developed in our previous studies [3-8]. In this work, structure and composition of La<sub>0.6</sub>Ca<sub>0.4</sub>Co<sub>0.5</sub>Fe<sub>0.5</sub>O<sub>3-d</sub> (LCCF) hollow fiber membranes were characterized before and after oxygen permeation tests in a CO<sub>2</sub> plasma. The oxygen permeation flux can be increased by one order of magnitude via this new plasma-assisted hollow fiber membrane concept, reaching up to 4 ml min<sup>-1</sup> cm<sup>-2</sup> in a CO<sub>2</sub> containing atmosphere. A constant high oxygen permeation flux was maintained during long-term operation, which is of major importance for commercial application. The applied rapid switching between operation and stand-by demonstrated the additional strength of the setup to cope with a potential unstable supply when using renewable electricity. These results show that plasma-assisted CO<sub>2</sub> conversion combined with a LCCF hollow fiber membrane allows to simultaneously enhance oxygen permeation and CO<sub>2</sub> conversion by inhibiting the reverse reactions. Therefore, it may be considered as a future industrial procedure for the autarkic formation of C1 platform chemicals from CO<sub>2</sub> and (excess) regenerative energy.

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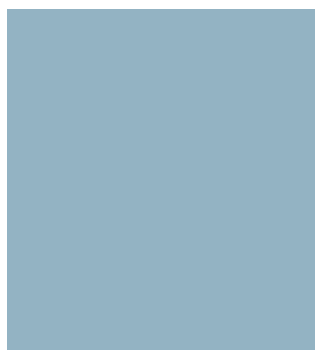
# Poster Sessions

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**Tim de la Croix**

## Upcycling of waste polyolefins via heterogeneous transfer dehydrogenation and olefin metathesis



*Tim de la Croix*  
*KU Leuven, Belgium*

Polyethylene (PE) is the most abundant plastic today, found in many single-use packaging applications, and therefore a major component of plastic waste streams (PlasticsEurope, 2022). Mechanical recycling of PE faces issues such as polymer degradation and contamination, making it difficult to achieve true circularity. Recently, novel methods for the catalytic upcycling of PE to e.g. propylene and telechelic macromonomers attracted significant attention (Conk et al., 2022; Arroyave et al., 2022). These methods start from partially unsaturated PE, prepared using a costly homogeneous Ir-pincer catalyst.

In this work, the use of simple and recoverable heterogeneous Pt catalysts is investigated for the preparation of partially unsaturated PE, using ethylene as an abundant and convenient hydrogen acceptor. At mild temperatures compared to classical dehydrogenations (< 300°C), dehydrogenation degrees between 0.5% and 1% of ethylene units can be achieved with minimal degradation of the polymer and high selectivity. The unsaturated polymer can be used as a substrate for tandem isomerization/metathesis to yield propylene, or in cross-metathesis to yield telechelic macromonomers, using commercially available Hoveyda-Grubbs catalysts.

To avoid the use of toxic acrylates, more benign olefins like dimethyl maleate and 1,4-diacetoxybutene are investigated for cross-metathesis, to yield methyl ester- or acetate-terminated telechelics respectively. Alternatively, versatile vinyl-terminated telechelics could be obtained via ethenolysis. Telechelic macromonomers could be repolymerized into polyethylene-like materials or incorporated into block-co-polymers for e.g. compatibilization of mixed plastic waste during mechanical recycling.

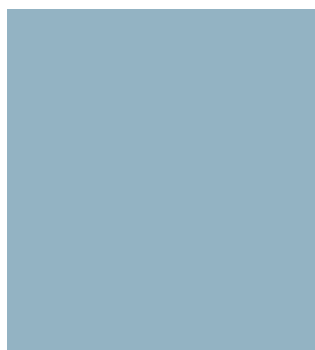
Thus, the partially unsaturated PE serves as a highly versatile intermediate for the upcycling of polyolefin waste to a variety of telechelic macromonomers and propylene. The heterogeneous transfer dehydrogenation of PE provides a simple method for the production of this intermediate, making chemical upcycling of plastic waste more accessible and contributing to a circular economy.

# Poster Sessions

P32

Ann-Katrin Emmerich

## Material development for a sustainable circular economy: A life cycle assessment of the synthesis methods of activators for the pyrolysis-catalysis of plastic waste in Germany



Ann-Katrin Emmerich  
TU Darmstadt

Addressing global crises like climate change and biodiversity loss necessitates comprehensive strategies, with a focus on circular economy principles e.g., for an effective plastic recycling strategy. The significance of a circular economy is demonstrated by its important contribution to the carbon cycle, ecosystem health, human well-being, biodiversity, and socio-economic resilience [1]. This importance prompted the introduction of Germany's »Circular Economy Act« in 2012. Despite legislative efforts, the majority of plastic waste (53% in 2021 [2]) in Germany is still energetically utilized, meaning incinerated, thereby eliminated from the recyclable resource loop.

To combat this issue, the pyrolysis-catalysis process offers a viable solution for chemical recycling of plastic waste [3,4]. In this process, polymers undergo thermal breakdown, and the resulting pyrolysis gas is converted into hydrogen gas and functional carbon material with the assistance of an activator. This activator is synthesized in a pre-form, where the catalyst particles, typically transition metals, are integrated into the structure. During the pyrolysis-catalysis, the activators decompose, leaving behind a support material decorated with evenly distributed transition metal nanoparticles. This approach holds promise due to its ability to offer a large surface area for the catalytically active sites. Several materials show potential for this application, including perovskites like LCCF ( $\text{La}_{1-x}\text{Ca}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_3-d$ ) [3], Mn-based spinels with transition metal cations [4], single-atom "catalysts" on polymer-derived ceramics (PDC), MXene-based catalysts, and red mud, a waste product from aluminum production. The careful selection of the respective activator material allows to steer the relation between gaseous, liquid (oil), and solid product phases, hence enabling chemical recycling of plastic waste, in particular of mixed fractions or polymer composite products [3,5]. However, recycling is not directly synonymous with sustainability. Thus, developing these materials requires consideration of both functionality and environmental impacts. Conducting a life cycle assessment (LCA) is crucial to be able to quantify the latter. Employing the ILCD 2011 Midpoint+ impact assessment method, the study examines various impact categories recommended by the EU [6]. The assessment focuses on the first part of the life cycle, encompassing raw material procurement to activator synthesis. Additionally, activator efficiency is considered by adjusting the required activator amount. Since research is still in its preliminary phase, the scope is confined to laboratory-scale experimentation. Nevertheless, this initial assessment provides valuable insights into the environmental footprints of respective materials and synthesis methods, guiding decisions towards materials that combine functionality with sustainability.

[1] Synthesis report of the IPCC sixth assessment report (AR6), 20 March 2023

[2] „Stoffstrombild Kunststoffe in Deutschland 2021: Zahlen und Fakten zum Lebensweg von Kunststoffen“ Studie, Conversio Market & Strategy GmbH, Oktober 2022

[3] X. Yu et al., App. Cat. B: Environmental 334 (2023) 122838

[4] X. Liu et al., App. Cat. B: Environmental 324 (2023) 122271

[5] R. Mishra et al., ACS Sustain. Chem. Eng. 11 (2023) 2033-2049

[6] <https://eplca.jrc.ec.europa.eu/uploads/LCIA-characterization-factors-of-the-ILCD.pdf>

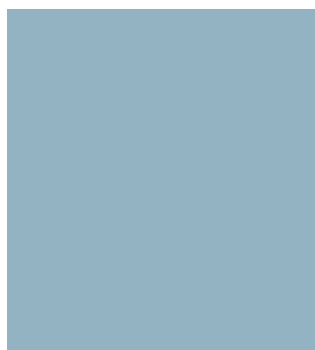
# Poster Sessions

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**Xiao Yu**

## Plasma Pyrolysis for Sustainable Plastic Waste Upcycling



*Xiao Yu*  
*Fraunhofer IWKS*

The substantial demand for plastics in daily life has led to a consistent and exponential increase in global production over the past few decades. The COVID-19 pandemic further enhanced the consumption of medical plastic materials, which are used to produce single-use health protection products. The current disposal routes for the post-customer wastes are mainly thermal utilization and landfill, which is environmentally unfriendly. More efficient and sustainable recycling methods are highly needed. Non-thermal plasma technologies have gained a lot of attention and are particularly appealing for quickly and efficiently converting waste plastics into valuable chemicals and materials. In this study, an atmospheric pressure microwave plasma was combined with perovskite-type pre-catalysts for the co-production of H<sub>2</sub> and value-added carbon composite materials. Different types of real-world plastic wastes have been tested with and without a pre-catalyst including high-density polyethylene, low-density polyethylene, polypropylene and polystyrene. For both thermal catalytic and plasma catalytic processes, the effect of different process parameters and pre-catalyst types on gas production and carbon species was thoroughly investigated. The physicochemical characteristics of the produced carbon nanomaterials were comprehensively characterized by the state-of-the-art techniques to investigate the relationship between the quantity and quality of carbon materials and plastic wastes types. Coupling thermal catalytic process with microwave plasma discharge resulted in a significant improvement of the H<sub>2</sub> yield. The presented findings demonstrated that the developed pre-catalyst is a promising candidate for the productions of H<sub>2</sub> and the carbon nanotube composites for energy storage applications from plastics in an atmospheric pressure microwave discharge.

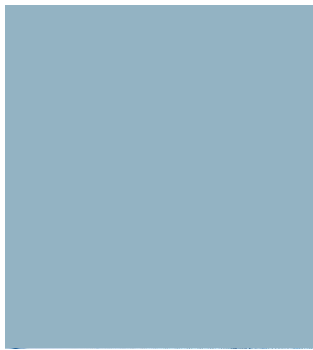
# Poster Sessions

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David Fahz

## K3I Cycling: An AI-based approach towards circular economy of plastic packaging



David Fahz  
Fraunhofer IWKS

The overall objective of K3I Cycling is to significantly improve the mechanical recycling of post-consumer plastic packaging waste, both quantitatively and qualitatively, and thus to enable the sustainable use of plastics in both industrial and private everyday life. This goes hand in hand with the aim of increasing the acceptance of products made from recycled materials among manufacturers and consumers. In order to achieve this goal, the following two key points will be addressed in the innovation lab: By creating and providing a new, open and standardizable artificial intelligence (AI) interface for the cross-sector collection of relevant information in terms of a light packaging (LVP) product passport, the digital networking of all stakeholders along the LVP value chain will be enabled for the first time. Building on the collected data and applying AI methods, the optimization of the entire LVP cycle is then addressed. Here, both the AI-based optimization of the processes in the individual sectors (logistics, sorting, processing, regranulation/recycling, etc.) as well as the AI-based overarching optimization of the entire value chain play significant role. The approach is realized by establishing an Artificial Neural Twin (ANT). This is a fully differentiable digital representation that has the ability to optimally adjust the individual components, and thus the overall system, to a global quality measure, while taking local conditions into account. In order to be able to develop the planned work on an industrial scale, the described points will be developed and optimized using an LVP sorting plant in real operation. Thus, a direct implementation is guaranteed, which is at the same time a strength and special feature of this project.



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